

**A method for performing restrained dynamics docking of one or multiple  
substrates on multi-specific enzymes**

5 The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multispecific and flexible active site. It also concerns a method for determining the 3D-structure of active sites that are flexible and can adapt to different substrates, which is the case for multispecific enzymes such as cytochrome  
10 P450.

As of today, various computer graphics systems allow to generate molecular models of large molecules such as proteins from the PDB structural data obtained using X-ray crystallography and NMR. We can cite for example MODELLER, COMPOSER, MATCHMAKER (Tripos), or 3D graphical environments for  
15 molecular modeling such as SYBYL (Tripos) or INSIGHT II (Accelrys).

Substrates as well as inhibitors or agonists often act by binding to particular regions of an enzyme or receptor referred as the active site. In industry, the purpose of using these 3D models is to assess the main features of the molecules which are involved in the binding to the active site. New molecules that fit the active site can be  
20 designed.

Biological interactions are not possible without flexibility and motion. One of the principal tools in the theoretical study of motion in biological molecules is the method of molecular dynamics simulations (MD). This computational method calculates the time dependent behavior of a molecular system (Karplus and  
25 McCammon, 2002). MD simulations have provided detailed information on the fluctuations and conformational changes of proteins and nucleic acids. These methods are now routinely used to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes. They are also used in the determination of structures from x-ray crystallography and from NMR  
30 experiments. The molecular dynamics simulations can be used to recreate the successive events in the binding process of a molecule, and thermodynamic parameters implicated in such process can therefore be derived, which is of great interest in the design of active molecules.

Nevertheless, the methods proposed in the art are based on a relatively low level of calculations of few parameters. It relies only on the molecule energy constrained with a fixed geometry. It relies only on the interaction energy between the molecule and the active site frozen in a fixed geometry.

- 5 Consequently, there is a need for a model replicating *in silico* the natural process of molecular interactions.

The method according to the invention provides both minimizations and molecular dynamics calculations. More specifically, it provides a new approach which is more appropriate to flexible structures, hereafter referred as “restrained dynamics  
10 docking” or “soft-restrained restrained dynamics docking”. This technique employs constrained dynamics simulations, where the only constraints are active site-substrate distances.

For example, to explain and predict drug metabolism in organisms, in which the cytochrome P450 (CYP) superfamily of haem-thiolate enzymes plays a central role,  
15 it is of large interest to dispose of a molecular picture of the binding sites responsible for the biotransformation. Efficiency of the prediction is then directly related to the molecular precision of the model, which resolution must be obtained at the atomic level to exploit the model for further docking studies.

In mammalian, hepatic cytochrome P450s constitute the major enzymes involved in  
20 the metabolism of exogenic compounds. Among them, isozymes of the CYP3 family (such as CYP3A1 and 3A2 in rat, and CYP3A4, CYP3A5, CYP3A7, CYP3A43 in human) are known to metabolize the majority of drugs in clinical use. These are multi-specific enzymes, able to metabolize a large variety of structurally diverse chemicals or substrates including steroids, linear or cyclized peptides  
25 (Delaforge et al. 1997, Delaforge et al. 2001, Aninat et al. 2001), generally fairly lipophilic, within a broad range of molecular sizes from testosterone (Mw 288) to cyclosporin A (Mw 1203).

The inventory of known substrates for CYP 3A contains a large variety of different molecules having apparently no common structural factors. Actually it can be  
30 estimated that more than five hundred utilized drugs can be recognized and metabolized by CYP 3A (Guengerich 1995, Wrighton et al. 2000, Lewis 2001). Closer inspection of the precise transformations catalyzed by CYP 3A indicates that there is an important regio- and stereo-selectivity for each substrate. The active site

can accommodate relatively rigid substrates such as aflatoxin derivatives or steroids, that are oxidized almost exclusively at a precise position. Thus CYP 3A4 catalyzes the testosterone oxidation exclusively at the 6 $\beta$  position, whereas CYP 3A7 oxidizes dehydroepiandrosterone (DHEA) or its 3 sulfate conjugate  
5 exclusively on the 16 $\alpha$  position (see Figures 4A and 4B). In addition to such small substrates, CYP 3A metabolize also large molecules such as cyclosporin A (MW 1202), macrolide antibiotics (MW around 600) or ergot derivatives (MW from 500 to 700).

The recognized substrates can have endogenous origin such as steroids or can be  
10 drugs or compounds found in food. For example, grapefruit juice contains bergamottin derivatives having specific CYP 3A inhibitory activities (Schmiedlin-Ren et al. 1997). Linear peptides (Delaforge et al. 2001, Hosea et al. 2000) or cyclized peptides (Delaforge et al. 1997) containing from 2 aminoacids (called diketopiperazine, Delaforge et al. 2001, Aninat et al. 2001) to 11 amino-acids (*e.g.*  
15 cyclosporin) are also recognized.

Following this wide range substrate recognition, a tentative subclassification was established leading to a multi-site hypothesis (Hosea et al. 2000, Ekins et al. 2003) consisting of at least 2 or 3 binding zones in the active site. This hypothesis has been established on the facts that CYP 3A shows often atypical hyperbolic kinetic  
20 constants and is thus unable to reach saturation. In addition, the presence in the active site of a second substrate having a different molecular nature lead to either no modification or increased metabolism of both substrates. Such allosteric effects have been clearly described in the case of simultaneous metabolism of steroids such as testosterone and  $\alpha$ -naphthoflavone.

25 Consequently, any molecular model describing correctly the multiple substrate specificity (that takes into account large variations in molecular size and chemical structures), and substrate cooperativity effects within the active site (when two or more drugs interact), is of considerable scientific and industrial interest. Such a molecular model must be able to rationalize the binding of the diverse known  
30 substrates, and the orientations of the molecules in the binding site that account for their known positions of metabolism (such as N-demethylations, benzylic hydroxylations etc.).

CYP3A4 is considered as the main hepatic form and is found in a wide variety of human organs such as intestine, brain or skin. CYP 3A5 is also present in liver and is the major 3A form present in the kidney. The 3A5 isoform is subject to genetic polymorphism. CYP 3A7 is the major 3A isoform present in the foetus whereas  
5 CYP3A43 is mainly located in adult prostate or testis. These isoforms share amino acid identities higher than 70%. (Westlind-Johnsson et al. 2003, Gellner et al. 2001, Koch et al. 2002). It is currently accepted that CYP3A4 is the most active isoform for classical P450 3A substrates whereas recent data (Williams et al. 2002) demonstrate equal or slightly reduced activity for CYP3A5 and a significantly  
10 lower metabolism capability for CYP3A7 as compared to CYP3A4. Additionally, differences have been observed in term of oxidative regioselectivity of the CYP3A7 compared to other isoforms. As an example, CYP3A7 metabolizes intensively DHEA and especially its sulfate conjugate derivative whereas CYP3A4 is a poor metabolizer. The oxidation by CYP3A7 occurs mostly in the 16 $\alpha$  position of  
15 DHEA. In contrast, CYP3A7 metabolizes testosterone in both 6 $\beta$  and 16 $\alpha$  position whereas CYP3A4 or 3A5 metabolize it almost exclusively in the 6 $\beta$  position (Inoue et al. 2000).

At the contrary of the P450 3A subfamily, other P450 isoforms have more rigid active site, as suggested by the narrow range of recognized substrates or inhibitors.  
20 These P450 isoforms recognize generally a small number of substrates or inhibitors having in common the same shape (i.e. P450 1A isoforms), or the same charge (i.e. CYP 2B, 2C or 2D isoforms), or the same chemical nature such as steroids (i.e. CYP19 or CYP21 isoforms) or lipids (i.e. CYP 4 family).

As no high-resolution 3D structure of CYP3A is today publicly available, due to  
25 continuing difficulties in promoting crystallization of intrinsic membrane proteins or due to an unusual conformational flexibility that would explain how CYP3A can accommodate various substrates, it is necessary to rebuild a 3D model structure, integrating the known biochemical data of CYP3A and the structural data of other members of the CYP superfamily. X-ray crystallographic determinations of several  
30 bacterial P450 enzymes in the 1990s (see Table 1 for a summary of structural data) have stimulated numerous attempts in modeling microsomal P450S such as human CYP3A4. The chapter 6 of the book "Guide to Cytochromes P450: structure and function" written by David F.V. Lewis reviews the current status of structural and



modeling investigations of the P450 family (Lewis 2001). This review was however written just before the release of the first mammalian P450 structure (2C5), still today the only one mammalian template available.

**Table 1**

| CYP isoform crystallized                     | PDB code (resol.) | Organism  | Function   | No of residues | Reference                                      |
|--|-------------------|---|--|----------------|--|
| P450 cam<br>(complexed by CO+camphor)        | 3cpp<br>(1.9 Å)   | <i>Pseudomonas Putida</i>                         | Camphor Monooxygenase  | 414            | (Poulos et al. 1985)<br>(Raag and Poulos 1989) |
| P450 terp                                    | 1cpt<br>(2.3 Å)   | <i>Pseudomonas</i> sp.                            | Alpha-terpineol hydroxylation  | 412            | (Hasemann et al. 1994)                         |
| P450 BM3                                     | 2hpd<br>(2 Å)     | <i>Bacillus megaterium</i>                        | Fatty acid monooxygenase   | 471            | (Ravichandran et al. 1993)                     |
| P450 cryF<br>(6-deoxyerythro-nolide B bound) | 1oxa<br>(2.1 Å)   | <i>Saccharopolyspora erythraea</i>                | Erythromycin biosynthesis 6S-hydroxylation of 6-deoxyerythronolide B | 403            | (Cupp-Vickery and Poulos 1995)                 |
| P450 nor                                     | 1rom<br>(2 Å)     | <i>Fusarium oxysporum</i> (denitrifying fungus)   | Nitric Oxide Reductase   | 403            | (Park et al. 1997)                             |
| P450 2C5                                     | 1dt6<br>(3 Å)     | (membrane-type Mammalian) Rabbit                  | Progesterone 21-Hydroxylase  | 473 (487)      | (Williams et al. 2000)                         |
| P450 CYP119<br>4-Phenylimidazole Bound       | 1f4t<br>(1.93 Å)  | <i>Sulfolobus Solfactarius</i> Thermophilic bact. | unknown  | 368            | (Yano et al. 2000)                             |
| P450 CYP51<br>4-Phenylimidazole Bound        | 1e9x<br>(2.1 Å)   | <i>Mycobacterium Tuberculosis</i>                 | 14 $\alpha$ -sterol demethylase                                      | 455 (451)      | (Podust et al. 2001)                           |

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Table 1: the eight X-ray crystal structures of P450s available in 2002: six bacterial, one fungal (P450 nor), one mammalian (CYP2C5). The P450<sub>cam</sub>, P450<sub>terp</sub>, P450<sub>cryF</sub>, P450<sub>nor</sub> belong to class I P450s enzymes, whereas P450<sub>BM3</sub> belongs to class II enzymes, like microsomal enzymes CYP2C5 and 3A. P450<sub>BM3</sub> structure is therefore  
10 *a priori* more relevant to rebuilding a structural model of CYP3A, but since the CYP2C5 X-Ray structure has been released, it became obvious that the structural homology between the other bacterial enzymes and microsomal enzymes was better than expected from the poor homology of primary structure (< 25% identity). Then, the relevance of using class I and class II structures together for rebuilding models  
15 of class II P450s was no more questionable. In the two examples described in the present invention, the structural model of human CYP3A4 was rebuilt using the six

first structures listed above, with no preference in the structural alignment, and the structural model of human CYP3A7 was rebuilt using four structures among those listed above with again no preference in the structural alignment, *i.e.* P450<sub>BM3</sub>, P450 EryF, P450 2C5 and CYP51, one of the last published structural sets. CYP119 was not incorporated into the modeling process.

All the proposed models of CYP3A4 obtained by homology modeling are thus so far based on bacterial crystal structure templates: the first was proposed by Ferenczy and Morris and used the X-ray structure of bacterial P450<sub>cam</sub> as unique template structure (Ferenczy and Morris 1989). Another model was built later by David F.V. Lewis, using also a unique template structure, the P450<sub>BM3</sub> structure, which was supposed to be more relevant as a template since this P450 was the only one class II enzyme with known three-dimensional structure (Lewis et al. 1996). A third model, based on a multiple structure template, was built by Szklarz and Halpert, using the four first X-ray crystal structures available P450<sub>cam</sub>, P450<sub>terp</sub>, P450<sub>eryF</sub>, and P450<sub>BM3</sub>. This four-bacterial template approach strategy is closer to our rebuilding strategy, but was still missing some relevance in the absence of a mammalian template. In our hands, the incorporation of the mammalian 2C5 crystal structure into rebuilding steps of models of cytochrome P450 3A proved to be decisive. Inclusion of 2C5 crystal structure had indeed a profound effect on the structural alignment with the five non-mammalian structures, resulting in a different topology of the active site and a marked divergence between the model and each individual template. The advantage of our multiple-template approach resides essentially in the availability of a final template that can be used to rebuild various mammalian cytochromes P450. Up to now there is no available crystal structure or structural model of human CYP3A5, CYP 3A7, CYP3A43 or other mammalian CYP3A.

More recently, two new bacterial P450 crystal structures emerged in the literature (Table 1): CYP51 (PDB code 1e9x), from *Mycobacterium tuberculosis*, that catalyzes the oxidative removal of 14 $\alpha$ -methyl group from sterol precursors in sterol biosynthesis in yeast and fungi (ergosterol), plants (phytosterol) and mammals (cholesterol), for its potential in the design of antifungal agents (Podust et al. 2001). And CYP119 (PDB code 1f4t), from the thermophilic archaeon *Sulfolobus solfataricus*, the first P450 identified in *Archaea*, for its interest in

understanding the enhanced thermal stability of the structure, especially in the region of the active site (Yano et al. 2000). Those two structures have been shown to exhibit the typical bacterial P450 fold, with some exceptions in the topology. They have not been included as structural templates in the modeling steps of the CYP3A4 model described in example 1. The names of newly discovered P450s follow the now accepted nomenclature of David R. Nelson (Nelson 1999).

The protein databank (Brookhaven Protein Databank, <http://www.rcsb.org/pdb/>) currently indicates that there are 76 separate crystal structures available for the eight crystallized P450s, plus 7 crystal structures on hold (Sept 1<sup>st</sup>, 2002), the majority of which containing either bound substrates or inhibitors. Table 1 provides the relevant information about the structural templates used for human CYP3A model rebuilding. The idea behind homology modeling is that proteins belonging to the same functional class and showing a strong sequence identity, adopt a similar fold (review in (Hilbert et al. 1993)). Known analogous structures are then used to generate a template or parent structure for the unknown protein to be modeled. The reliability of the various methods employed depend mostly on the number of experimental 3D structures that can be aligned. Knowing that for pairs of distantly related proteins (with residue identity of about 20%) the regions having the same fold will represent less than half of each molecule, the regions where the folds differ will predominate, and the divergence of sequence must be compensated by a higher number of homologous proteins to align (Chothia and Lesk 1986). Below 50% of sequence identity, the deviation in structurally not conserved regions becomes significant, and loop regions are difficult to predict. It is generally accepted that below 20% of sequence identity, the prediction turns out to be hazardous, and fold assignment methods are best replaced by *ab initio* methods, that ideally attempt to predict the native structure only from the primary sequence of the protein to be modeled. But produced models so far had the correct fold for only a few small protein domains (Sanchez et al. 2000).

The strategy of model rebuilding in the P450 family is strongly driven by the low degree of homology between bacterial and mammal cytochrome P450s (Table 2).

Table 2

| PDB code | Swiss-Prot entry name  | CP37_ HUMAN      | CP34_ HUMAN      | CP51_ MYCTU      | CPXW_ SULSO      | CPC5_ RABIT      | CPXA_ PSEPU      | CPXL_ PSESP      | CPXB_ BACME      | CPXJ_ SACER      | NOR_ FUSOX |
|----------|------------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------|
| n.s.     | CP37_HUMAN             | 88.4 %<br>372 aa |                  |                  |                  |                  |                  |                  |                  |                  |            |
| n.s.     | CP34_HUMAN             | 88.4 %<br>372 aa | 50.1 aa          |                  |                  |                  |                  |                  |                  |                  |            |
| 1E9X     | CP51_MYCTU (CYP51)     | 27.7 %<br>372 aa | 26.9 %<br>405 aa |                  |                  |                  |                  |                  |                  |                  |            |
| 1F4T     | CPXW_SULSO (CYP119)    | 24.5 %<br>330 aa | 25.4 %<br>410 aa | 25.7 %<br>385 aa |                  |                  |                  |                  |                  |                  |            |
| 1DT6     | CPC5_RABIT (CYP2C5)    | 27.9 %<br>481 aa | 28.4 %<br>497 aa | 23.4 %<br>427 aa | 23.5 %<br>344 aa |                  |                  |                  |                  |                  |            |
| 3CPP     | CPXA_PSEPU (P450 cam)  | 23.3 %<br>335 aa | 21.3 %<br>399 aa | 21.9 %<br>407 aa | 26.6 %<br>387 aa | 24.2 %<br>480 aa |                  |                  |                  |                  |            |
| ICPT     | CPXL_PSESP (P450 terp) | 24.8 %<br>452 aa | 24.4 %<br>356 aa | 27.8 %<br>446 aa | 29.3 %<br>409 aa | 24.4 %<br>451 aa | 27.4 %<br>398 aa |                  |                  |                  |            |
| 2HPD-A   | CPXB_BACME (P450 BM3)  | 31.8 %<br>409 aa | 29.9 %<br>445 aa | 27.1 %<br>443 aa | 24.5 %<br>396 aa | 22.7 %<br>480 aa | 23.1 %<br>485 aa | 24.0 %<br>363 aa |                  |                  |            |
| 10XA     | CPXJ_SACER (P450 eryF) | 25.5 %<br>415 aa | 26.0 %<br>334 aa | 27.7 %<br>423 aa | 30.8 %<br>396 aa | 24.4 %<br>443 aa | 24.0 %<br>391 aa | 28.6 %<br>420 aa | 22.6 %<br>389 aa |                  |            |
| 1ROM     | NOR_FUSOX (P450 nor)   | 23.7 %<br>354 aa | 22.9 %<br>415 aa | 23.1 %<br>442 aa | 27.7 %<br>379 aa | 21.4 %<br>351 aa | 29.0 %<br>379 aa | 31.5 %<br>409 aa | 23.0 %<br>265 aa | 32.7 %<br>395 aa |            |

Table 2: Sequence identities between the various crystallized cytochrome P450s and human CYP3A4 and CYP3A7 using BLOSUM 62 matrix (source LALIGN, [http://www.infobiogen.fr/services/analyseq/cgi-bin/lfastap\\_in.pl](http://www.infobiogen.fr/services/analyseq/cgi-bin/lfastap_in.pl), algorithm of

- 5 Huang and Miller LALIGN that finds the best local alignments between two sequences, version 2.1u03 April 2000, published in *Adv. Appl. Math.* 1991, 12 : 373-381). The P450 BM3 structure, Swissprot code name CPXB\_BACME, corresponds to the structure of a fusion protein of P450 and a reductase domain, so that it displays twice the number of residues.
- 10 Our global scheme, which steps are described hereafter, is founded on a combination of methods developed in the literature for different purposes in protein structure determination studies. The principle of the primary steps, until the generation of a correct alignment of P450 primary sequences, is described in Jean et al. 1997. The last steps are summarized in Loiseau 2002.
- 15 Therefore, in a first object, the invention relates to a method for designing a 3-dimensional (3-D) model of a protein, the 3-D representation of at least three family members has already been experimentally obtained, [said 3-D representation presenting similarities], comprising the steps of:
- a. identification of common structural blocks (CSBs) among said members of said
  - 20 family,
  - b. alignment of the amino-acids primary sequence of said family members according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
  - c. alignment of said protein as compared on said first alignment, in order to obtain a
  - 25 second alignment, wherein:
    - i. alignment of said protein is performed in order to optimize the amino-acids alignment between said protein and said first alignment,  
when one or more consensus amino-acid exists in said aligned CSBs in said first alignment, and in the amino-acid sequence of said protein, said consensus
    - 30 amino-acids are anchors of said second alignment,
    - ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible in out-of-block regions, if better to align the primary amino-acids sequences,

- d. definition of the 3-D structure of CSBs of said protein, according to the 3-D structure of the CSBs of said family members,
- e. definition of the global constraints (distance and angular constraints) derived from the comparisons of the structural templates in CSBs, and definition of the local constraints (distance and angular constraints) for the atoms of residues that are not structurally determined after step d. (that are not in the CSBs),
- f. selection of rotamers,
- g. determination of a family of 3-D model structures of said protein, taking into account said 3-D structure of CSBs obtained in step d., said global and local constraints defined in step e., and said rotamers defined in step f.,
- h. optimization of said family of 3-D models obtained in step g., by
  - i discarding structures that present topological defects, and
  - ii recalculating 3-D structures by taking electrostatic forces into account, and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment, when the obtained model structures do not satisfactorily account for known mutations having biological effects.

In the present invention, the term "backbone atoms" refers to the C, N, C $\alpha$ , and O atoms of a protein that are common to all amino acid building blocks or involved in the peptide linkage. When the protein structure is described as a trajectory in internal coordinates such as  $\alpha$ ,  $\tau$  angles, or is a low-resolution crystallographic structure, backbone atoms stand only for C $\alpha$  atoms of each residue.

In the present invention, the term "similarities" is used in the search for structural fragments conserved between the template proteins, that is fragments that have similar local trajectories in the backbone internal coordinate space. Two protein fragments have "similar" local trajectories when they are matched according to two adjustable parameters, the mesh and the margin (Jean et al. 1997).

In the present invention, the term "common structural blocks (CSB)" define the protein fragments of equal length that are found similar between all the template proteins in the internal coordinate representation.

In the present invention, the term "first alignment" refers to the alignment imposed by the CSBs, that is the structural alignment between template proteins defined by

CSBs sequences. This alignment is totally independent on the primary sequence of the template proteins.

In the present invention, the term "out-of-block regions" designates all other protein fragments located out of and between the CSBs, *i.e.* that are not structurally conserved in the internal coordinate space. There is no information of sequence alignment for these regions (see in Figure 1 regions that are not colored), since they are not relevant for structural conservation. Out-of-block regions are passively reconstructed with the rest of the structure during the calculation steps.

In the present invention, the term "global constraints" refers to geometric constraints that are assigned to atoms of residues from CSBs, and that can be derived by computing all distance or angle information available within CSBs or between CSB.

In the present invention, the term "local constraints" refers to loose structural constraints that are assigned to residues of out-of-block regions, in order to restrict their backbone conformation to allowed regions of the Ramachandran diagram.

In the present invention, the term "rotamers" defines the low energy side-chain conformations of residues. The use of a library of rotamers allows determining or modeling a structure with the most likely side-chain conformations, saving time and producing a structure that is more likely to be correct.

For identification of CSBs between all selected 3D structures:

CSBs define the common local folds found similar in the template proteins, and are used as building blocks to set up the fold of the model (results in Loiseau 2002). The non conserved regions, that can be parts of secondary structures or non-structured regions as loops, will be rebuilt with no initial structural information.

For multiple alignment of crystalline P450s, on the basis of CSBs determination:

Once the structurally conserved elements are identified, a first structural alignment between the template proteins is derived. The following step involves the localization of these elements in the target sequence. Sequence pairwise comparisons between selected crystal structures and CYP3A (Table 2) show low sequence identity, so that online tools of multiple alignment such as CLUSTALW or PHD (Heidelberg) fail to produce an clear-cut alignment. Instead, local alignment tools, such as that described in Jean et al. 1997, were used to match the CSB profile to the target sequence, where a matrix is slid along the sequence and a

score of similarity (based on a standard matrix such as BLOSUM62) is calculated for each position. Online tools of multiple alignment such as CLUSTALW 1.8 can be further used for assessment of accuracy.

The target sequence of human cytochrome P450 3A is thus aligned against the multiple alignment obtained from the CSBs. This produces the key sequence alignment which allows the generation of the template structure used for the rebuilding of the various CYP3A models. Following steps involve:

- 1) Generation of distance and dihedral angles constraints.
- 2) Selection of rotamers for side chains in CSBs.
- 10 3) Calculation of a set of structures using DYANA software. Loops are rebuilt between CSBs.
- 4) Structure optimization under XPLOR software (Brünger 1992).

In a preferred embodiment, said 3-D representation of family members has been obtained by crystallography or NMR.

- 15 The alignment of said common structural blocks in steps b. and c. can be performed by use of the GOK software as described in Jean et al., 1997.

In addition, step d. is preferably performed according to the following rules:

- i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues  
20 are purely assigned to the target residue,
- ii. When residues differ, only the coordinates of the backbone atoms are assigned (C $\alpha$ ), and sometimes C $\beta$  or C $\gamma$  when they exist.

The definition of rebuilding global constraints in step e. is performed by using all available geometrical information intra- and inter-CSB (distances and angles),  
25 issued from the comparisons of the structural templates, each geometric constraint being defined as an interval. On another hand, the definition of local constraints for out-of-blocks residues is performed by analysis of the allowed regions in Ramachandran diagram.

Furthermore, distances and angles defining global constraints are preferably  
30 selected in step e. by the following rules:

- i. all distances for which the lower boundary is less than 8 Å,
- ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs



iii. all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom.

The distance of 8 Å is chosen in order to reduce drastically the total number of constraints to take into account in the computation, and to allow to excessively  
5 constrain the model.

Angular constraints are preferably selected in step e. by the following rule:

i. dihedral angles  $\phi$  and  $\psi$  of all residues located in CSBs are defined as constraints, given by the average values of corresponding  $\phi$ ,  $\psi$  angles in said  
10 family members +/- the calculated standard deviation.

To practice the method of the invention, rotamers in step f. can be selected from the couples according to the tables of Dunbrack and Karplus and step g. can be performed with the DYANA software, as described in Güntert et al, 1997.

In addition, the optimization in step h. comprises the use of the X-Plor software, as  
15 described in A. T. Brünger, X-PLOR, version 3.1.

The method according to the invention is particularly applicable to a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A]

In a preferred embodiment, said mammal cytochrome P450 3A is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29  
20 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).

In another preferred embodiment, said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).

The method is applicable as well to human cytochrome of the subfamily P450 3A4,  
25 wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A4 are chosen from Nor (SEQ ID N° 1), Ery F (SEQ ID N° 2), terp (SEQ ID N° 3), Cam (SEQ ID N° 4), BM3 (SEQ ID N° 5) and 2C5 (SEQ ID N° 6).

The method is applicable as well to human cytochrome of the subfamily 3A7,  
30 wherein family members that are used for performing said first alignment for designing a 3-D model of CYP3A7 are chosen from Ery F (SEQ ID N° 2), BM3 (SEQ ID N° 5), CYP51 (SEQ ID N° 8) and 2C5 (SEQ ID N° 6).

The method is applicable as well to other mammalian cytochrome P450 3A isoforms.

In a second object, the invention is directed to 3-D structure model of a protein, obtained by the method as described above.

- 5 In a preferred embodiment, the protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A

In another preferred embodiment, the protein is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).

- 10 In still another preferred embodiment, the protein is a human cytochrome P450 subfamily 3A selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).  
In still another preferred embodiment, the protein is a human cytochrome P450 3A4 or 3A7.

- 15 Regarding the rebuilt P450 3A4 model, the main residues involved in the recognition of the substrate are **C97; R104; F101; F107; F247; F303 and C376**.  
More specifically, C97 and C376 are found in positions compatible with the formation of a disulfide bridge allowing limited or enhanced flexibility of corresponding protein domains, while R104 is involved in the capture of the  
20 substrate that is close to the entrance site, and allows to accompany it to the active site. F303 is involved in the recognition of the substrate in the active site. F107; F247 and F303 are involved in the recognition at the modulation site responsible for positive regulation. Role of F303 in the active site has already been suggested by studies of Domanski et al. 1998 in the SRS 4 region (mutants I300, F303, A304,  
25 and T308).

Features of this model comprise the 3-D atomic coordinates of **Table 3**.

#### Table 3

- In a preferred embodiment, the residues C97; R104; F101; F107; F247; F303 and C376 are involved in the CYP 3A4 for the recognition and uptake of the substrate at  
30 the entry site, and its binding into the active site having the 3-D atomic coordinates of Table 3.

Regarding the P450 3A7 model, features comprise the 3-D atomic coordinates of **Table 4**.

Table 4

In a preferred embodiment the residues Q79; F102; R105; R106; F108; F248; F304 and E374 are involved in the CYP 3A7 for the recognition and uptake of the substrate at the entry site, and its binding into the active having the 3-D atomic  
5 coordinates of Table 4.

In a third object, the invention contemplates a method for designing a protein, biological functions of which are altered, comprising:

- a) obtaining a 3-D model of said protein by the method as depicted above,
- b) analyzing said model of step a., and determining the amino-acids that are  
10 putatively involved in the biological functions of said protein,
- c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.

In the present invention, the term "altered properties" means that the generated  
15 protein is altered in its enzymatic properties, such as the substrate recognition, the movements associated to the entrance or the exit of the substrate, the multiple binding at the active site, the allosteric behaviour, the electron transfer, the coupling to the P450 reductase.

In another object, the invention relates to a computer-assisted method for  
20 performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps:

- j. determining a force field, and independently simulating the presence of said enzyme in said force field,
- k. minimizing the potential energy ( $E_p$ ) linked to said force field of said 3-D  
25 structure, wherein the spatial position of some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by
  - i. simulating an increase in temperature (in order to give kinetic energy),
  - ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- 30 l. optionally repeating step k in order to obtain other  $E_p$  minima, wherein said  $E_p$  minima are such that the structure of the protein remains folded,
- m. minimizing  $E_p$  in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by

- i. simulating an increase in temperature (in order to give kinetic energy), and
- ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- n. simulating, at 0 K the presence of said substrate next to said enzyme,
- o. optionally generating a molecular dynamics simulation on said substrate and enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)
- p. generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- q. generating a molecular dynamics simulation on said substrate and enzyme, with said constraints imposed in step p.,
- r. optionally, generating a molecular dynamics simulation on said substrate and enzyme without said constraints of step p.

In the present invention, the term "restrained dynamics docking" means a procedure by which the docking of the substrate is simulated using molecular dynamics (MD) simulations under constraints that are specified by the user.

In the present invention, the term "soft-restrained dynamics docking" refers to a restrained dynamics docking in which the substrate-protein distance constraints are loose, with force field parameters associated to the constraints as low as 1 or 2 Kcal/mol.

- 20 In the present invention, the term "constraints" when applied to substrate docking refers to a distance imposed between atoms of the protein, generally from the active site (such as atoms of the heme group), and atoms of the substrate. These distance restraints are defined as intervals, where the distance range is large enough to allow the free movement of the substrate within the active site.
- 25 In a preferred embodiment of this method for performing restrained dynamics docking, said fixed atoms in step k. are the backbone atoms N-C $\alpha$ -CO in the first minimization step and only C $\alpha$  in subsequent minimization steps.

In another preferred embodiment of this method, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

- 30 The force field in step j. comprises forces linked to:
- a. the distance between atoms,
  - b. the angles of valence,
  - c. the dihedral angles,

- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- g. hydrogen bonds.

- 5 The constraints in step **p.** are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- 10 In the present invention, the term "final distance constraints", when applied to substrate docking, means distances imposed between atoms from the heme group (such as the iron atom), and atoms of the substrate. These distance constraints are defined as intervals, and are related to the final position of the substrate in the vicinity of the heme group before metabolization.
- 15 Preferably, step **o.** is performed with a simulated temperature of between about 15 and 50 K, step **q.** is performed with a simulated temperature of between about 15 and 50 K, and step **r.** is performed with a simulated temperature of between about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome 36

- 20 P450 subfamily 3A comprising mammal and human cytochromes.

The cytochrome can be cytochrome P450 3A4 or any of all other P450 from the 3A subfamily, and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.

- 25 The substrate can be a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).

In a preferred embodiment said substrate is testosterone.

In another object, the invention is aimed at a computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a  
30 3-D structure of which is available, consisting of performing the steps **j, k, l, m, n, o, p, q and r** depicted above with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained state after molecular dynamics simulations.

The first and second substrates can be the same molecule or different molecules.

The first and second substrates can display either allosteric or synergistic effect.

This method can be practiced with substrates that are inhibitors (competitive, uncompetitive, non competitive) or display an inhibitor-base mechanism. It can also

5 be practiced with an agonist and any molecule interfering with the biological function of the protein.

In preferred embodiments:

- the first and second substrates are the same molecule.
- the first and second substrates are different molecules.
- 10 - the first and second substrates display an allosteric effect.
- the first and second substrates display a synergistic effect.
- at least one of the substrates is an inhibitor or display an inhibitor-based mechanism.
- at least one of the substrates is an agonist.

15 In another embodiment, this method also embraces a successive repeat of the steps j, k, l, m, n, o, p, q and r depicted above with a 3<sup>rd</sup>, 4<sup>th</sup> or 5<sup>th</sup> substrate, some of them being the same or different molecules.

In this method for performing restrained dynamics docking, said fixed atoms in step k. are the backbone atoms N-C $\alpha$ -CO in the first minimization step and only C $\alpha$  in  
20 subsequent minimization steps.

In addition, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

The force field in step j. comprises preferably forces linked to

- a. the distance between atoms,
- 25 b. the angles of valence,
- c. the dihedral angles,
- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- 30 g. hydrogen bonds.

The constraints in step p. are preferable attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance

constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.

Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome P450. The cytochrome can be cytochrome P450 3A4, or any of all other P450 of the 3A subfamily and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.

In a preferred embodiment:

- said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the above-described method, in particular the above-described model structure,
- said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A),
- said substrate is testosterone.

The invention is also directed to the use of the method for designing a 3-D model of a protein and to the computer-assisted method for performing restrained dynamics docking as mentioned above for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.

Another object of the invention is the use of these methods for determining the effect of a first substrate on a second substrate, which can also be applied to pharmaceutical products.

The invention contemplates the use of these methods for determining the effect of a first bound testosterone molecule on the access of a second testosterone molecule as well as for determining the mutual effect of a testosterone molecule with alpha-naphthoflavone ( $\alpha$ NF) molecule.

The invention is also directed to :

- \* The use of the above described computer-assisted methods for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate to give rise to metabolite.  
The oxidized or reduced molecule derived from a given substrate modified after positioning at the right distance to the heme is called metabolite.
- \* The use of the above described computer-assisted methods, for performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the calculation.
- \* The use of the above described computer-assisted methods for dynamic docking to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to determine if the exit of the given metabolite from the enzyme is favored or not.
- \* The use of the above described computer-assisted methods for dynamic docking to study the different exit pathways that are accessible to the metabolite, either in the absence or in the presence of the second substrate in the calculation.

The distance and angular constraints derived from CSBs common to the crystallized cytochromes P450 used as structural templates, are applied to conserved atoms of CSBs of the target protein. The DYANA software (Güntert et al. 1997) allows to rebuild directly the whole structure of the target protein on the basis of its primary sequence, by taking into account these geometric constraints. Out-of-blocks residues are rebuilt *ab initio* by selecting the most favorable solutions in terms of minimal global potential energy. As examples, actual tables 3 and 4 display the atomic coordinates of structural models obtained by applying DYANA calculation to target protein sequences CYP3A4 and CYP3A7 respectively.



TABLE 3 :Providing the coordinates of the CYP3A4 model

|        |  |  |     |     |        |        |        |      |      |     |     |     |     |     |     |
|--------|--|--|-----|-----|--------|--------|--------|------|------|-----|-----|-----|-----|-----|-----|
| HEADER | CYP3A4   |  |     |     |        |        |        |      |      |     |     |     |     |     |     |
| TITLE  | MODEL OF HUMAN CYTOCHROME P450 CYP3A4            |  |     |     |        |        |        |      |      |     |     |     |     |     |     |
| AUTHOR | N. LOISEAU, F. ANDRE, C. MINOLETTI, M. DELAFORGE |  |     |     |        |        |        |      |      |     |     |     |     |     |     |
| SEQRES | 1  | 452  | SER | TYR | HIS    | LYS    | GLY    | PHE  | CYS  | MET | PHE | ASP | MET | GLU | CYS |
| SEQRES | 2  | 452  | HIS | LYS | LYS    | TYR    | GLY    | LYS  | VAL  | TRP | GLY | PHE | TYR | ASP | GLY |
| SEQRES | 3  | 452  | GLN | GLN | PRO    | VAL    | LEU    | ALA  | ILE  | THR | ASP | PRO | ASP | MET | ILE |
| SEQRES | 4  | 452  | LYS | THR | VAL    | LEU    | VAL    | LYS  | GLU  | CYS | TYR | SER | VAL | PHE | THR |
| SEQRES | 5  | 452  | ASN | ARG | ARG    | PRO    | PHE    | GLY  | PRO  | VAL | GLY | PHE | MET | LYS | SER |
| SEQRES | 6  | 452  | ALA | ILE | SER    | ILE    | ALA    | GLU  | ASP  | GLU | GLU | TRP | LYS | ARG | LEU |
| SEQRES | 7  | 452  | ARG | SER | LEU    | LEU    | SER    | PRO  | THR  | PHE | THR | SER | GLY | LYS | LEU |
| SEQRES | 8  | 452  | LYS | GLU | MET    | VAL    | PRO    | ILE  | ILE  | ALA | GLN | TYR | GLY | ASP | VAL |
| SEQRES | 9  | 452  | LEU | VAL | ARG    | ASN    | LEU    | ARG  | ARG  | GLU | ALA | GLU | THR | GLY | LYS |
| SEQRES | 10   | 452  | PRO | VAL | THR    | LEU    | LYS    | ASP  | VAL  | PHE | GLY | ALA | TYR | SER | MET |
| SEQRES | 11   | 452  | ASP | VAL | ILE    | THR    | SER    | THR  | SER  | PHE | GLY | VAL | ASN | ILE | ASP |
| SEQRES | 12   | 452  | SER | LEU | ASN    | ASN    | PRO    | GLN  | ASP  | PRO | PHE | VAL | GLU | ASN | THR |
| SEQRES | 13   | 452  | LYS | LYS | LEU    | LEU    | ARG    | PHE  | ASP  | PHE | LEU | ASP | PRO | PHE | PHE |
| SEQRES | 14   | 452  | LEU | SER | ILE    | THR    | VAL    | PHE  | PRO  | PHE | LEU | ILE | PRO | ILE | LEU |
| SEQRES | 15   | 452  | GLU | VAL | LEU    | ASN    | ILE    | CYS  | VAL  | PHE | PRO | ARG | GLU | VAL | THR |
| SEQRES | 16   | 452  | ASN | PHE | LEU    | ARG    | LYS    | SER  | VAL  | LYS | ARG | MET | LYS | GLU | SER |
| SEQRES | 17   | 452  | ARG | LEU | GLU    | ASP    | THR    | GLN  | LYS  | HIS | ARG | VAL | ASP | PHE | LEU |
| SEQRES | 18   | 452  | GLN | LEU | MET    | ILE    | ASP    | SER  | GLN  | ASN | SER | LYS | GLU | THR | GLU |
| SEQRES | 19   | 452  | SER | HIS | LYS    | ALA    | LEU    | SER  | ASP  | LEU | GLU | LEU | VAL | ALA | GLN |
| SEQRES | 20   | 452  | SER | ILE | ILE    | PHE    | ILE    | PHE  | ALA  | GLY | TYR | GLU | THR | THR | SER |
| SEQRES | 21   | 452  | SER | VAL | LEU    | SER    | PHE    | ILE  | MET  | TYR | GLU | LEU | ALA | THR | HIS |
| SEQRES | 22   | 452  | PRO | ASP | VAL    | GLN    | GLN    | LYS  | LEU  | GLN | GLU | GLU | ILE | ASP | ALA |
| SEQRES | 23   | 452  | VAL | LEU | PRO    | ASN    | LYS    | ALA  | PRO  | PRO | THR | TYR | ASP | THR | VAL |
| SEQRES | 24   | 452  | LEU | GLN | MET    | GLU    | TYR    | LEU  | ASP  | MET | VAL | VAL | ASN | GLU | THR |
| SEQRES | 25   | 452  | LEU | ARG | LEU    | PHE    | PRO    | ILE  | ALA  | MET | ARG | LEU | GLU | ARG | VAL |
| SEQRES | 26   | 452  | CYS | LYS | LYS    | ASP    | VAL    | GLU  | ILE  | ASN | GLY | MET | PHE | ILE | PRO |
| SEQRES | 27   | 452  | LYS | GLY | TRP    | VAL    | MET    | ILE  | PRO  | SER | TYR | ALA | LEU | HIS |     |
| SEQRES | 28   | 452  | ARG | ASP | PRO    | LYS    | TYR    | TRP  | THR  | GLU | PRO | GLU | LYS | PHE | LEU |
| SEQRES | 29   | 452  | PRO | GLU | ARG    | PHE    | SER    | LYS  | LYS  | ASN | LYS | ASP | ASN | ILE | ASP |
| SEQRES | 30   | 452  | PRO | TYR | ILE    | TYR    | THR    | PRO  | PHE  | GLY | SER | GLY | PRO | ARG | ASN |
| SEQRES | 31   | 452  | CYS | ILE | GLY    | MET    | ARG    | PHE  | ALA  | LEU | MET | ASN | MET | LYS | LEU |
| SEQRES | 32   | 452  | ALA | LEU | ILE    | ARG    | VAL    | LEU  | GLN  | ASN | PHE | SER | PHE | LYS | PRO |
| SEQRES | 33   | 452  | CYS | LYS | GLU    | THR    | GLN    | ILE  | PRO  | LEU | LYS | LEU | SER | LEU | GLY |
| SEQRES | 34   | 452  | GLY | LEU | LEU    | GLN    | PRO    | GLU  | LYS  | PRO | VAL | VAL | LEU | LYS | VAL |
| SEQRES | 35   | 452  | GLU | SER | ARG    | ASP    | GLY    | THR  | VAL  | SER | GLY | ALA |     |     |     |
| HET    | HEM  | 600  |     |     |        |        |        |      |      |     |     |     |     |     |     |
| HETNAM | HEM  | HEME   |     |     |        |        |        |      |      |     |     |     |     |     |     |
| HETSYN | HEM  | 3,7,12,17-TETRAMETHYL-8,13-DIVINYL-2,18-PORPHINEDIPROPIONIC ACID |     |     |        |        |        |      |      |     |     |     |     |     |     |
| FORMUL | HEM  | C34 H34 N4 O4 FE1  |     |     |        |        |        |      |      |     |     |     |     |     |     |
| ATOM   | 1  | N  | SER | 51  | 9.999  | -1.760 | -4.543 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 2  | CA   | SER | 51  | 10.718 | -0.477 | -4.293 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 3  | CB   | SER | 51  | 9.949  | 0.731  | -4.939 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 4  | OG   | SER | 51  | 8.601  | 0.876  | -4.493 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 5  | C  | SER | 51  | 10.962 | -0.281 | -2.815 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 6  | O  | SER | 51  | 10.277 | -0.855 | -1.969 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 7  | N  | TYR | 52  | 11.974 | 0.569  | -2.482 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 8  | CA   | TYR | 52  | 12.433 | 0.860  | -1.131 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 9  | CB   | TYR | 52  | 13.983 | 0.783  | -0.979 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 10   | CG   | TYR | 52  | 14.459 | -0.572 | -1.430 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 11   | CD1  | TYR | 52  | 14.143 | -1.732 | -0.699 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 12   | CD2  | TYR | 52  | 15.210 | -0.701 | -2.611 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 13   | CE1  | TYR | 52  | 14.574 | -2.994 | -1.138 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 14   | CE2  | TYR | 52  | 15.651 | -1.954 | -3.052 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 15   | CZ   | TYR | 52  | 15.334 | -3.105 | -2.314 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 16   | OH   | TYR | 52  | 15.784 | -4.370 | -2.751 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 17   | C  | TYR | 52  | 11.971 | 2.246  | -0.755 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 18   | O  | TYR | 52  | 12.178 | 3.208  | -1.494 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 19   | N  | HIS | 53  | 11.321 | 2.350  | 0.429  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 20   | CA   | HIS | 53  | 10.747 | 3.568  | 0.953  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 21   | ND1  | HIS | 53  | 7.857  | 1.850  | 1.039  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 22   | CG   | HIS | 53  | 8.485  | 2.636  | 0.097  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 23   | CB   | HIS | 53  | 9.322  | 3.861  | 0.386  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 24   | NE2  | HIS | 53  | 7.438  | 0.923  | -0.936 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 25   | CD2  | HIS | 53  | 8.216  | 2.053  | -1.104 | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 26   | CE1  | HIS | 53  | 7.247  | 0.842  | 0.368  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 27   | C  | HIS | 53  | 10.751 | 3.386  | 2.448  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 28   | O  | HIS | 53  | 9.715  | 3.183  | 3.080  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |
| ATOM   | 29   | N  | LYS | 54  | 11.973 | 3.461  | 3.043  | 1.00 | 0.00 |     |     |     |     |     | 3A4 |

|      |     |     |     |    |        |        |        |      |      |     |
|------|-----|-----|-----|----|--------|--------|--------|------|------|-----|
| ATOM | 30  | CA  | LYS | 54 | 12.265 | 3.262  | 4.451  | 1.00 | 0.00 | 3A4 |
| ATOM | 31  | CB  | LYS | 54 | 13.401 | 2.217  | 4.659  | 1.00 | 0.00 | 3A4 |
| ATOM | 32  | CG  | LYS | 54 | 13.053 | 0.819  | 4.120  | 1.00 | 0.00 | 3A4 |
| ATOM | 33  | CD  | LYS | 54 | 14.220 | -0.183 | 4.148  | 1.00 | 0.00 | 3A4 |
| ATOM | 34  | CE  | LYS | 54 | 14.793 | -0.500 | 5.540  | 1.00 | 0.00 | 3A4 |
| ATOM | 35  | NZ  | LYS | 54 | 13.763 | -1.087 | 6.431  | 1.00 | 0.00 | 3A4 |
| ATOM | 36  | C   | LYS | 54 | 12.660 | 4.603  | 5.025  | 1.00 | 0.00 | 3A4 |
| ATOM | 37  | O   | LYS | 54 | 13.829 | 4.851  | 5.317  | 1.00 | 0.00 | 3A4 |
| ATOM | 38  | N   | GLY | 55 | 11.656 | 5.510  | 5.181  | 1.00 | 0.00 | 3A4 |
| ATOM | 39  | CA  | GLY | 55 | 11.819 | 6.901  | 5.560  | 1.00 | 0.00 | 3A4 |
| ATOM | 40  | C   | GLY | 55 | 11.464 | 7.113  | 7.003  | 1.00 | 0.00 | 3A4 |
| ATOM | 41  | O   | GLY | 55 | 10.305 | 7.002  | 7.400  | 1.00 | 0.00 | 3A4 |
| ATOM | 42  | N   | PHE | 56 | 12.502 | 7.439  | 7.817  | 1.00 | 0.00 | 3A4 |
| ATOM | 43  | CA  | PHE | 56 | 12.451 | 7.714  | 9.250  | 1.00 | 0.00 | 3A4 |
| ATOM | 44  | CB  | PHE | 56 | 13.646 | 7.051  | 10.010 | 1.00 | 0.00 | 3A4 |
| ATOM | 45  | CG  | PHE | 56 | 13.966 | 5.681  | 9.448  | 1.00 | 0.00 | 3A4 |
| ATOM | 46  | CD1 | PHE | 56 | 15.250 | 5.415  | 8.926  | 1.00 | 0.00 | 3A4 |
| ATOM | 47  | CD2 | PHE | 56 | 12.987 | 4.669  | 9.370  | 1.00 | 0.00 | 3A4 |
| ATOM | 48  | CE1 | PHE | 56 | 15.543 | 4.185  | 8.320  | 1.00 | 0.00 | 3A4 |
| ATOM | 49  | CE2 | PHE | 56 | 13.271 | 3.445  | 8.747  | 1.00 | 0.00 | 3A4 |
| ATOM | 50  | CZ  | PHE | 56 | 14.550 | 3.205  | 8.224  | 1.00 | 0.00 | 3A4 |
| ATOM | 51  | C   | PHE | 56 | 12.446 | 9.211  | 9.542  | 1.00 | 0.00 | 3A4 |
| ATOM | 52  | O   | PHE | 56 | 11.957 | 9.670  | 10.570 | 1.00 | 0.00 | 3A4 |
| ATOM | 53  | N   | CYS | 57 | 12.971 | 10.054 | 8.624  | 1.00 | 0.00 | 3A4 |
| ATOM | 54  | CA  | CYS | 57 | 13.048 | 11.500 | 8.782  | 1.00 | 0.00 | 3A4 |
| ATOM | 55  | CB  | CYS | 57 | 13.902 | 12.161 | 7.665  | 1.00 | 0.00 | 3A4 |
| ATOM | 56  | SG  | CYS | 57 | 15.312 | 11.121 | 7.176  | 1.00 | 0.00 | 3A4 |
| ATOM | 57  | C   | CYS | 57 | 11.705 | 12.171 | 8.760  | 1.00 | 0.00 | 3A4 |
| ATOM | 58  | O   | CYS | 57 | 11.446 | 13.160 | 9.434  | 1.00 | 0.00 | 3A4 |
| ATOM | 59  | N   | MET | 58 | 10.778 | 11.585 | 7.975  | 1.00 | 0.00 | 3A4 |
| ATOM | 60  | CA  | MET | 58 | 9.402  | 12.000 | 7.870  | 1.00 | 0.00 | 3A4 |
| ATOM | 61  | CB  | MET | 58 | 8.715  | 11.289 | 6.694  | 1.00 | 0.00 | 3A4 |
| ATOM | 62  | CG  | MET | 58 | 9.360  | 11.641 | 5.343  | 1.00 | 0.00 | 3A4 |
| ATOM | 63  | SD  | MET | 58 | 8.469  | 11.004 | 3.887  | 1.00 | 0.00 | 3A4 |
| ATOM | 64  | CE  | MET | 58 | 8.922  | 9.256  | 4.080  | 1.00 | 0.00 | 3A4 |
| ATOM | 65  | C   | MET | 58 | 8.612  | 11.706 | 9.122  | 1.00 | 0.00 | 3A4 |
| ATOM | 66  | O   | MET | 58 | 7.740  | 12.480 | 9.487  | 1.00 | 0.00 | 3A4 |
| ATOM | 67  | N   | PHE | 59 | 8.963  | 10.612 | 9.844  | 1.00 | 0.00 | 3A4 |
| ATOM | 68  | CA  | PHE | 59 | 8.394  | 10.230 | 11.122 | 1.00 | 0.00 | 3A4 |
| ATOM | 69  | CB  | PHE | 59 | 8.732  | 8.752  | 11.449 | 1.00 | 0.00 | 3A4 |
| ATOM | 70  | CG  | PHE | 59 | 7.865  | 8.152  | 12.538 | 1.00 | 0.00 | 3A4 |
| ATOM | 71  | CD1 | PHE | 59 | 6.477  | 8.002  | 12.350 | 1.00 | 0.00 | 3A4 |
| ATOM | 72  | CD2 | PHE | 59 | 8.430  | 7.747  | 13.764 | 1.00 | 0.00 | 3A4 |
| ATOM | 73  | CE1 | PHE | 59 | 5.671  | 7.462  | 13.364 | 1.00 | 0.00 | 3A4 |
| ATOM | 74  | CE2 | PHE | 59 | 7.627  | 7.208  | 14.780 | 1.00 | 0.00 | 3A4 |
| ATOM | 75  | CZ  | PHE | 59 | 6.247  | 7.065  | 14.579 | 1.00 | 0.00 | 3A4 |
| ATOM | 76  | C   | PHE | 59 | 8.881  | 11.119 | 12.255 | 1.00 | 0.00 | 3A4 |
| ATOM | 77  | O   | PHE | 59 | 8.110  | 11.479 | 13.139 | 1.00 | 0.00 | 3A4 |
| ATOM | 78  | N   | ASP | 60 | 10.162 | 11.568 | 12.226 | 1.00 | 0.00 | 3A4 |
| ATOM | 79  | CA  | ASP | 60 | 10.690 | 12.515 | 13.200 | 1.00 | 0.00 | 3A4 |
| ATOM | 80  | CB  | ASP | 60 | 12.225 | 12.651 | 13.131 | 1.00 | 0.00 | 3A4 |
| ATOM | 81  | CG  | ASP | 60 | 12.906 | 11.313 | 13.450 | 1.00 | 0.00 | 3A4 |
| ATOM | 82  | OD1 | ASP | 60 | 12.613 | 10.736 | 14.532 | 1.00 | 0.00 | 3A4 |
| ATOM | 83  | OD2 | ASP | 60 | 13.743 | 10.859 | 12.624 | 1.00 | 0.00 | 3A4 |
| ATOM | 84  | C   | ASP | 60 | 10.102 | 13.900 | 13.031 | 1.00 | 0.00 | 3A4 |
| ATOM | 85  | O   | ASP | 60 | 9.841  | 14.603 | 14.000 | 1.00 | 0.00 | 3A4 |
| ATOM | 86  | N   | MET | 61 | 9.809  | 14.318 | 11.780 | 1.00 | 0.00 | 3A4 |
| ATOM | 87  | CA  | MET | 61 | 9.130  | 15.564 | 11.481 | 1.00 | 0.00 | 3A4 |
| ATOM | 88  | CB  | MET | 61 | 9.224  | 15.881 | 9.987  | 1.00 | 0.00 | 3A4 |
| ATOM | 89  | CG  | MET | 61 | 10.590 | 16.349 | 9.497  | 1.00 | 0.00 | 3A4 |
| ATOM | 90  | SD  | MET | 61 | 10.659 | 16.502 | 7.686  | 1.00 | 0.00 | 3A4 |
| ATOM | 91  | CE  | MET | 61 | 12.223 | 17.411 | 7.689  | 1.00 | 0.00 | 3A4 |
| ATOM | 92  | C   | MET | 61 | 7.653  | 15.548 | 11.870 | 1.00 | 0.00 | 3A4 |
| ATOM | 93  | O   | MET | 61 | 7.073  | 16.551 | 12.274 | 1.00 | 0.00 | 3A4 |
| ATOM | 94  | N   | GLU | 62 | 7.012  | 14.358 | 11.819 | 1.00 | 0.00 | 3A4 |
| ATOM | 95  | CA  | GLU | 62 | 5.653  | 14.159 | 12.272 | 1.00 | 0.00 | 3A4 |
| ATOM | 96  | CB  | GLU | 62 | 5.077  | 12.770 | 11.933 | 1.00 | 0.00 | 3A4 |
| ATOM | 97  | CG  | GLU | 62 | 4.640  | 12.657 | 10.462 | 1.00 | 0.00 | 3A4 |
| ATOM | 98  | CD  | GLU | 62 | 4.351  | 11.190 | 10.120 | 1.00 | 0.00 | 3A4 |
| ATOM | 99  | OE1 | GLU | 62 | 3.429  | 10.603 | 10.748 | 1.00 | 0.00 | 3A4 |
| ATOM | 100 | OE2 | GLU | 62 | 5.048  | 10.637 | 9.227  | 1.00 | 0.00 | 3A4 |
| ATOM | 101 | C   | GLU | 62 | 5.522  | 14.338 | 13.751 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |    |        |        |        |      |      |     |
|------|-----|-----|-----|----|--------|--------|--------|------|------|-----|
| ATOM | 102 | O   | GLU | 62 | 4.508  | 14.819 | 14.225 | 1.00 | 0.00 | 3A4 |
| ATOM | 103 | N   | CYS | 63 | 6.605  | 14.104 | 14.522 | 1.00 | 0.00 | 3A4 |
| ATOM | 104 | CA  | CYS | 63 | 6.664  | 14.441 | 15.921 | 1.00 | 0.00 | 3A4 |
| ATOM | 105 | CB  | CYS | 63 | 7.902  | 13.805 | 16.588 | 1.00 | 0.00 | 3A4 |
| ATOM | 106 | SG  | CYS | 63 | 7.977  | 11.995 | 16.382 | 1.00 | 0.00 | 3A4 |
| ATOM | 107 | C   | CYS | 63 | 6.526  | 15.952 | 16.211 | 1.00 | 0.00 | 3A4 |
| ATOM | 108 | O   | CYS | 63 | 6.277  | 16.322 | 17.335 | 1.00 | 0.00 | 3A4 |
| ATOM | 109 | N   | HIS | 64 | 6.436  | 16.853 | 15.182 | 1.00 | 0.00 | 3A4 |
| ATOM | 110 | CA  | HIS | 64 | 5.487  | 17.970 | 15.236 | 1.00 | 0.00 | 3A4 |
| ATOM | 111 | ND1 | HIS | 64 | 4.140  | 20.440 | 16.744 | 1.00 | 0.00 | 3A4 |
| ATOM | 112 | CG  | HIS | 64 | 5.232  | 20.460 | 15.904 | 1.00 | 0.00 | 3A4 |
| ATOM | 113 | CB  | HIS | 64 | 6.151  | 19.284 | 15.666 | 1.00 | 0.00 | 3A4 |
| ATOM | 114 | NE2 | HIS | 64 | 4.280  | 22.506 | 15.939 | 1.00 | 0.00 | 3A4 |
| ATOM | 115 | CD2 | HIS | 64 | 5.301  | 21.731 | 15.420 | 1.00 | 0.00 | 3A4 |
| ATOM | 116 | CE1 | HIS | 64 | 3.608  | 21.687 | 16.726 | 1.00 | 0.00 | 3A4 |
| ATOM | 117 | C   | HIS | 64 | 4.780  | 18.138 | 13.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 118 | O   | HIS | 64 | 3.812  | 17.438 | 13.610 | 1.00 | 0.00 | 3A4 |
| ATOM | 119 | N   | LYS | 65 | 5.240  | 19.107 | 13.073 | 1.00 | 0.00 | 3A4 |
| ATOM | 120 | CA  | LYS | 65 | 4.699  | 19.426 | 11.766 | 1.00 | 0.00 | 3A4 |
| ATOM | 121 | CB  | LYS | 65 | 3.264  | 20.052 | 11.761 | 1.00 | 0.00 | 3A4 |
| ATOM | 122 | CG  | LYS | 65 | 2.994  | 21.171 | 12.783 | 1.00 | 0.00 | 3A4 |
| ATOM | 123 | CD  | LYS | 65 | 1.557  | 21.704 | 12.722 | 1.00 | 0.00 | 3A4 |
| ATOM | 124 | CE  | LYS | 65 | 1.220  | 22.723 | 13.820 | 1.00 | 0.00 | 3A4 |
| ATOM | 125 | NZ  | LYS | 65 | 2.052  | 23.944 | 13.700 | 1.00 | 0.00 | 3A4 |
| ATOM | 126 | C   | LYS | 65 | 5.705  | 20.365 | 11.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 127 | O   | LYS | 65 | 5.958  | 20.315 | 9.944  | 1.00 | 0.00 | 3A4 |
| ATOM | 128 | N   | LYS | 66 | 6.332  | 21.227 | 12.000 | 1.00 | 0.00 | 3A4 |
| ATOM | 129 | CA  | LYS | 66 | 7.517  | 22.020 | 11.730 | 1.00 | 0.00 | 3A4 |
| ATOM | 130 | CB  | LYS | 66 | 7.373  | 23.548 | 12.037 | 1.00 | 0.00 | 3A4 |
| ATOM | 131 | CG  | LYS | 66 | 6.519  | 24.352 | 11.039 | 1.00 | 0.00 | 3A4 |
| ATOM | 132 | CD  | LYS | 66 | 5.001  | 24.175 | 11.175 | 1.00 | 0.00 | 3A4 |
| ATOM | 133 | CE  | LYS | 66 | 4.191  | 25.119 | 10.278 | 1.00 | 0.00 | 3A4 |
| ATOM | 134 | NZ  | LYS | 66 | 2.736  | 24.881 | 10.442 | 1.00 | 0.00 | 3A4 |
| ATOM | 135 | C   | LYS | 66 | 8.551  | 21.370 | 12.620 | 1.00 | 0.00 | 3A4 |
| ATOM | 136 | O   | LYS | 66 | 9.100  | 20.332 | 12.253 | 1.00 | 0.00 | 3A4 |
| ATOM | 137 | N   | TYR | 67 | 8.772  | 21.934 | 13.838 | 1.00 | 0.00 | 3A4 |
| ATOM | 138 | CA  | TYR | 67 | 9.441  | 21.263 | 14.936 | 1.00 | 0.00 | 3A4 |
| ATOM | 139 | CB  | TYR | 67 | 11.005 | 21.348 | 14.926 | 1.00 | 0.00 | 3A4 |
| ATOM | 140 | CG  | TYR | 67 | 11.555 | 20.265 | 14.028 | 1.00 | 0.00 | 3A4 |
| ATOM | 141 | CD1 | TYR | 67 | 11.325 | 18.909 | 14.336 | 1.00 | 0.00 | 3A4 |
| ATOM | 142 | CD2 | TYR | 67 | 12.250 | 20.569 | 12.847 | 1.00 | 0.00 | 3A4 |
| ATOM | 143 | CE1 | TYR | 67 | 11.798 | 17.884 | 13.506 | 1.00 | 0.00 | 3A4 |
| ATOM | 144 | CE2 | TYR | 67 | 12.720 | 19.550 | 12.006 | 1.00 | 0.00 | 3A4 |
| ATOM | 145 | CZ  | TYR | 67 | 12.507 | 18.207 | 12.342 | 1.00 | 0.00 | 3A4 |
| ATOM | 146 | OH  | TYR | 67 | 13.010 | 17.184 | 11.509 | 1.00 | 0.00 | 3A4 |
| ATOM | 147 | C   | TYR | 67 | 8.880  | 21.880 | 16.194 | 1.00 | 0.00 | 3A4 |
| ATOM | 148 | O   | TYR | 67 | 8.905  | 23.092 | 16.404 | 1.00 | 0.00 | 3A4 |
| ATOM | 149 | N   | GLY | 68 | 8.343  | 20.969 | 17.043 | 1.00 | 0.00 | 3A4 |
| ATOM | 150 | CA  | GLY | 68 | 7.620  | 21.161 | 18.278 | 1.00 | 0.00 | 3A4 |
| ATOM | 151 | C   | GLY | 68 | 8.251  | 20.139 | 19.164 | 1.00 | 0.00 | 3A4 |
| ATOM | 152 | O   | GLY | 68 | 8.314  | 18.954 | 18.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 153 | N   | LYS | 69 | 8.864  | 20.642 | 20.260 | 1.00 | 0.00 | 3A4 |
| ATOM | 154 | CA  | LYS | 69 | 10.301 | 20.592 | 20.404 | 1.00 | 0.00 | 3A4 |
| ATOM | 155 | CB  | LYS | 69 | 10.795 | 21.997 | 20.802 | 1.00 | 0.00 | 3A4 |
| ATOM | 156 | CG  | LYS | 69 | 10.332 | 23.112 | 19.844 | 1.00 | 0.00 | 3A4 |
| ATOM | 157 | CD  | LYS | 69 | 10.770 | 24.527 | 20.225 | 1.00 | 0.00 | 3A4 |
| ATOM | 158 | CE  | LYS | 69 | 9.876  | 25.161 | 21.300 | 1.00 | 0.00 | 3A4 |
| ATOM | 159 | NZ  | LYS | 69 | 10.236 | 26.582 | 21.514 | 1.00 | 0.00 | 3A4 |
| ATOM | 160 | C   | LYS | 69 | 10.811 | 19.541 | 21.360 | 1.00 | 0.00 | 3A4 |
| ATOM | 161 | O   | LYS | 69 | 11.914 | 19.033 | 21.177 | 1.00 | 0.00 | 3A4 |
| ATOM | 162 | N   | VAL | 70 | 10.033 | 19.200 | 22.410 | 1.00 | 0.00 | 3A4 |
| ATOM | 163 | CA  | VAL | 70 | 10.427 | 18.227 | 23.408 | 1.00 | 0.00 | 3A4 |
| ATOM | 164 | CB  | VAL | 70 | 10.984 | 18.837 | 24.696 | 1.00 | 0.00 | 3A4 |
| ATOM | 165 | CG1 | VAL | 70 | 12.504 | 18.835 | 24.571 | 1.00 | 0.00 | 3A4 |
| ATOM | 166 | CG2 | VAL | 70 | 10.344 | 20.206 | 25.037 | 1.00 | 0.00 | 3A4 |
| ATOM | 167 | C   | VAL | 70 | 9.212  | 17.394 | 23.695 | 1.00 | 0.00 | 3A4 |
| ATOM | 168 | O   | VAL | 70 | 8.176  | 17.901 | 24.111 | 1.00 | 0.00 | 3A4 |
| ATOM | 169 | N   | TRP | 71 | 9.337  | 16.067 | 23.484 | 1.00 | 0.00 | 3A4 |
| ATOM | 170 | CA  | TRP | 71 | 8.255  | 15.133 | 23.636 | 1.00 | 0.00 | 3A4 |
| ATOM | 171 | CB  | TRP | 71 | 7.614  | 14.787 | 22.260 | 1.00 | 0.00 | 3A4 |
| ATOM | 172 | CG  | TRP | 71 | 6.390  | 13.874 | 22.229 | 1.00 | 0.00 | 3A4 |
| ATOM | 173 | CD2 | TRP | 71 | 5.135  | 14.145 | 22.880 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |    |        |        |        |      |      |     |
|------|-----|-----|-----|----|--------|--------|--------|------|------|-----|
| ATOM | 174 | CD1 | TRP | 71 | 6.251  | 12.660 | 21.615 | 1.00 | 0.00 | 3A4 |
| ATOM | 175 | NE1 | TRP | 71 | 4.996  | 12.146 | 21.846 | 1.00 | 0.00 | 3A4 |
| ATOM | 176 | CE2 | TRP | 71 | 4.292  | 13.040 | 22.624 | 1.00 | 0.00 | 3A4 |
| ATOM | 177 | CE3 | TRP | 71 | 4.695  | 15.227 | 23.643 | 1.00 | 0.00 | 3A4 |
| ATOM | 178 | CZ2 | TRP | 71 | 2.995  | 12.995 | 23.131 | 1.00 | 0.00 | 3A4 |
| ATOM | 179 | CZ3 | TRP | 71 | 3.388  | 15.180 | 24.153 | 1.00 | 0.00 | 3A4 |
| ATOM | 180 | CH2 | TRP | 71 | 2.551  | 14.080 | 23.902 | 1.00 | 0.00 | 3A4 |
| ATOM | 181 | C   | TRP | 71 | 8.828  | 13.911 | 24.261 | 1.00 | 0.00 | 3A4 |
| ATOM | 182 | O   | TRP | 71 | 9.989  | 13.584 | 24.059 | 1.00 | 0.00 | 3A4 |
| ATOM | 183 | N   | GLY | 72 | 7.987  | 13.188 | 25.027 | 1.00 | 0.00 | 3A4 |
| ATOM | 184 | CA  | GLY | 72 | 8.345  | 11.936 | 25.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 185 | C   | GLY | 72 | 7.812  | 10.809 | 24.804 | 1.00 | 0.00 | 3A4 |
| ATOM | 186 | O   | GLY | 72 | 6.679  | 10.850 | 24.336 | 1.00 | 0.00 | 3A4 |
| ATOM | 187 | N   | PHE | 73 | 8.645  | 9.773  | 24.586 | 1.00 | 0.00 | 3A4 |
| ATOM | 188 | CA  | PHE | 73 | 8.334  | 8.591  | 23.820 | 1.00 | 0.00 | 3A4 |
| ATOM | 189 | CB  | PHE | 73 | 9.278  | 8.443  | 22.586 | 1.00 | 0.00 | 3A4 |
| ATOM | 190 | CG  | PHE | 73 | 8.893  | 7.320  | 21.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 191 | CD1 | PHE | 73 | 9.691  | 6.162  | 21.549 | 1.00 | 0.00 | 3A4 |
| ATOM | 192 | CD2 | PHE | 73 | 7.717  | 7.398  | 20.877 | 1.00 | 0.00 | 3A4 |
| ATOM | 193 | CE1 | PHE | 73 | 9.320  | 5.105  | 20.707 | 1.00 | 0.00 | 3A4 |
| ATOM | 194 | CE2 | PHE | 73 | 7.344  | 6.343  | 20.030 | 1.00 | 0.00 | 3A4 |
| ATOM | 195 | CZ  | PHE | 73 | 8.146  | 5.196  | 19.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 196 | C   | PHE | 73 | 8.515  | 7.451  | 24.788 | 1.00 | 0.00 | 3A4 |
| ATOM | 197 | O   | PHE | 73 | 9.257  | 7.543  | 25.757 | 1.00 | 0.00 | 3A4 |
| ATOM | 198 | N   | TYR | 74 | 7.826  | 6.328  | 24.540 | 1.00 | 0.00 | 3A4 |
| ATOM | 199 | CA  | TYR | 74 | 7.884  | 5.174  | 25.397 | 1.00 | 0.00 | 3A4 |
| ATOM | 200 | CB  | TYR | 74 | 6.631  | 5.032  | 26.304 | 1.00 | 0.00 | 3A4 |
| ATOM | 201 | CG  | TYR | 74 | 5.298  | 5.291  | 25.625 | 1.00 | 0.00 | 3A4 |
| ATOM | 202 | CD1 | TYR | 74 | 4.515  | 4.223  | 25.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 203 | CD2 | TYR | 74 | 4.797  | 6.603  | 25.491 | 1.00 | 0.00 | 3A4 |
| ATOM | 204 | CE1 | TYR | 74 | 3.279  | 4.456  | 24.524 | 1.00 | 0.00 | 3A4 |
| ATOM | 205 | CE2 | TYR | 74 | 3.564  | 6.844  | 24.870 | 1.00 | 0.00 | 3A4 |
| ATOM | 206 | CZ  | TYR | 74 | 2.804  | 5.769  | 24.384 | 1.00 | 0.00 | 3A4 |
| ATOM | 207 | OH  | TYR | 74 | 1.560  | 6.006  | 23.757 | 1.00 | 0.00 | 3A4 |
| ATOM | 208 | C   | TYR | 74 | 8.100  | 4.007  | 24.486 | 1.00 | 0.00 | 3A4 |
| ATOM | 209 | O   | TYR | 74 | 7.256  | 3.682  | 23.658 | 1.00 | 0.00 | 3A4 |
| ATOM | 210 | N   | ASP | 75 | 9.272  | 3.357  | 24.603 | 1.00 | 0.00 | 3A4 |
| ATOM | 211 | CA  | ASP | 75 | 9.664  | 2.238  | 23.778 | 1.00 | 0.00 | 3A4 |
| ATOM | 212 | CB  | ASP | 75 | 11.110 | 2.479  | 23.220 | 1.00 | 0.00 | 3A4 |
| ATOM | 213 | CG  | ASP | 75 | 11.483 | 1.556  | 22.044 | 1.00 | 0.00 | 3A4 |
| ATOM | 214 | OD1 | ASP | 75 | 10.755 | 1.577  | 21.015 | 1.00 | 0.00 | 3A4 |
| ATOM | 215 | OD2 | ASP | 75 | 12.500 | 0.822  | 22.166 | 1.00 | 0.00 | 3A4 |
| ATOM | 216 | C   | ASP | 75 | 9.580  | 1.007  | 24.657 | 1.00 | 0.00 | 3A4 |
| ATOM | 217 | O   | ASP | 75 | 9.275  | 1.091  | 25.845 | 1.00 | 0.00 | 3A4 |
| ATOM | 218 | N   | GLY | 76 | 9.925  | -0.191 | 24.123 | 1.00 | 0.00 | 3A4 |
| ATOM | 219 | CA  | GLY | 76 | 10.101 | -1.403 | 24.908 | 1.00 | 0.00 | 3A4 |
| ATOM | 220 | C   | GLY | 76 | 11.420 | -1.335 | 25.643 | 1.00 | 0.00 | 3A4 |
| ATOM | 221 | O   | GLY | 76 | 12.463 | -1.562 | 25.039 | 1.00 | 0.00 | 3A4 |
| ATOM | 222 | N   | GLN | 77 | 11.349 | -0.928 | 26.946 | 1.00 | 0.00 | 3A4 |
| ATOM | 223 | CA  | GLN | 77 | 12.393 | -0.521 | 27.882 | 1.00 | 0.00 | 3A4 |
| ATOM | 224 | CB  | GLN | 77 | 13.760 | -1.300 | 27.835 | 1.00 | 0.00 | 3A4 |
| ATOM | 225 | CG  | GLN | 77 | 14.891 | -0.783 | 26.903 | 1.00 | 0.00 | 3A4 |
| ATOM | 226 | CD  | GLN | 77 | 15.977 | -1.843 | 26.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 227 | OE1 | GLN | 77 | 16.121 | -2.718 | 27.611 | 1.00 | 0.00 | 3A4 |
| ATOM | 228 | NE2 | GLN | 77 | 16.759 | -1.765 | 25.648 | 1.00 | 0.00 | 3A4 |
| ATOM | 229 | C   | GLN | 77 | 12.593 | 0.983  | 27.782 | 1.00 | 0.00 | 3A4 |
| ATOM | 230 | O   | GLN | 77 | 12.935 | 1.504  | 26.719 | 1.00 | 0.00 | 3A4 |
| ATOM | 231 | N   | GLN | 78 | 12.365 | 1.707  | 28.918 | 1.00 | 0.00 | 3A4 |
| ATOM | 232 | CA  | GLN | 78 | 12.698 | 3.105  | 29.188 | 1.00 | 0.00 | 3A4 |
| ATOM | 233 | CB  | GLN | 78 | 14.220 | 3.411  | 28.944 | 1.00 | 0.00 | 3A4 |
| ATOM | 234 | CG  | GLN | 78 | 14.774 | 4.789  | 29.381 | 1.00 | 0.00 | 3A4 |
| ATOM | 235 | CD  | GLN | 78 | 14.622 | 5.043  | 30.889 | 1.00 | 0.00 | 3A4 |
| ATOM | 236 | OE1 | GLN | 78 | 14.409 | 4.138  | 31.694 | 1.00 | 0.00 | 3A4 |
| ATOM | 237 | NE2 | GLN | 78 | 14.757 | 6.336  | 31.296 | 1.00 | 0.00 | 3A4 |
| ATOM | 238 | C   | GLN | 78 | 11.820 | 4.135  | 28.453 | 1.00 | 0.00 | 3A4 |
| ATOM | 239 | O   | GLN | 78 | 11.794 | 4.125  | 27.222 | 1.00 | 0.00 | 3A4 |
| ATOM | 240 | N   | PRO | 79 | 11.120 | 5.089  | 29.129 | 1.00 | 0.00 | 3A4 |
| ATOM | 241 | CA  | PRO | 79 | 10.604 | 6.330  | 28.550 | 1.00 | 0.00 | 3A4 |
| ATOM | 242 | CD  | PRO | 79 | 10.730 | 4.946  | 30.533 | 1.00 | 0.00 | 3A4 |
| ATOM | 243 | CB  | PRO | 79 | 9.535  | 6.798  | 29.557 | 1.00 | 0.00 | 3A4 |
| ATOM | 244 | CG  | PRO | 79 | 10.001 | 6.244  | 30.911 | 1.00 | 0.00 | 3A4 |
| ATOM | 245 | C   | PRO | 79 | 11.734 | 7.327  | 28.383 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |    |        |        |        |      |      |     |
|------|-----|-----|-----|----|--------|--------|--------|------|------|-----|
| ATOM | 246 | O   | PRO | 79 | 12.582 | 7.447  | 29.260 | 1.00 | 0.00 | 3A4 |
| ATOM | 247 | N   | VAL | 80 | 11.782 | 8.012  | 27.228 | 1.00 | 0.00 | 3A4 |
| ATOM | 248 | CA  | VAL | 80 | 12.870 | 8.876  | 26.835 | 1.00 | 0.00 | 3A4 |
| ATOM | 249 | CB  | VAL | 80 | 13.698 | 8.283  | 25.679 | 1.00 | 0.00 | 3A4 |
| ATOM | 250 | CG1 | VAL | 80 | 14.441 | 7.026  | 26.173 | 1.00 | 0.00 | 3A4 |
| ATOM | 251 | CG2 | VAL | 80 | 12.828 | 7.928  | 24.440 | 1.00 | 0.00 | 3A4 |
| ATOM | 252 | C   | VAL | 80 | 12.250 | 10.173 | 26.392 | 1.00 | 0.00 | 3A4 |
| ATOM | 253 | O   | VAL | 80 | 11.117 | 10.204 | 25.939 | 1.00 | 0.00 | 3A4 |
| ATOM | 254 | N   | LEU | 81 | 13.003 | 11.285 | 26.466 | 1.00 | 0.00 | 3A4 |
| ATOM | 255 | CA  | LEU | 81 | 12.603 | 12.575 | 25.948 | 1.00 | 0.00 | 3A4 |
| ATOM | 256 | CB  | LEU | 81 | 12.958 | 13.700 | 26.945 | 1.00 | 0.00 | 3A4 |
| ATOM | 257 | CG  | LEU | 81 | 12.302 | 15.079 | 26.699 | 1.00 | 0.00 | 3A4 |
| ATOM | 258 | CD1 | LEU | 81 | 10.822 | 15.078 | 27.116 | 1.00 | 0.00 | 3A4 |
| ATOM | 259 | CD2 | LEU | 81 | 13.057 | 16.197 | 27.437 | 1.00 | 0.00 | 3A4 |
| ATOM | 260 | C   | LEU | 81 | 13.352 | 12.751 | 24.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 261 | O   | LEU | 81 | 14.529 | 12.427 | 24.569 | 1.00 | 0.00 | 3A4 |
| ATOM | 262 | N   | ALA | 82 | 12.695 | 13.249 | 23.585 | 1.00 | 0.00 | 3A4 |
| ATOM | 263 | CA  | ALA | 82 | 13.260 | 13.415 | 22.267 | 1.00 | 0.00 | 3A4 |
| ATOM | 264 | CB  | ALA | 82 | 12.433 | 12.689 | 21.183 | 1.00 | 0.00 | 3A4 |
| ATOM | 265 | C   | ALA | 82 | 13.288 | 14.890 | 21.990 | 1.00 | 0.00 | 3A4 |
| ATOM | 266 | O   | ALA | 82 | 12.251 | 15.546 | 22.002 | 1.00 | 0.00 | 3A4 |
| ATOM | 267 | N   | ILE | 83 | 14.498 | 15.436 | 21.733 | 1.00 | 0.00 | 3A4 |
| ATOM | 268 | CA  | ILE | 83 | 14.742 | 16.837 | 21.486 | 1.00 | 0.00 | 3A4 |
| ATOM | 269 | CB  | ILE | 83 | 16.032 | 17.330 | 22.124 | 1.00 | 0.00 | 3A4 |
| ATOM | 270 | CG2 | ILE | 83 | 15.944 | 18.846 | 22.217 | 1.00 | 0.00 | 3A4 |
| ATOM | 271 | CG1 | ILE | 83 | 16.359 | 16.727 | 23.506 | 1.00 | 0.00 | 3A4 |
| ATOM | 272 | CD  | ILE | 83 | 15.380 | 17.044 | 24.634 | 1.00 | 0.00 | 3A4 |
| ATOM | 273 | C   | ILE | 83 | 14.831 | 17.000 | 19.986 | 1.00 | 0.00 | 3A4 |
| ATOM | 274 | O   | ILE | 83 | 15.706 | 16.418 | 19.358 | 1.00 | 0.00 | 3A4 |
| ATOM | 275 | N   | THR | 84 | 13.915 | 17.773 | 19.367 | 1.00 | 0.00 | 3A4 |
| ATOM | 276 | CA  | THR | 84 | 13.796 | 17.851 | 17.920 | 1.00 | 0.00 | 3A4 |
| ATOM | 277 | CB  | THR | 84 | 12.384 | 17.503 | 17.457 | 1.00 | 0.00 | 3A4 |
| ATOM | 278 | OG1 | THR | 84 | 11.371 | 18.330 | 18.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 279 | CG2 | THR | 84 | 12.085 | 16.027 | 17.808 | 1.00 | 0.00 | 3A4 |
| ATOM | 280 | C   | THR | 84 | 14.259 | 19.175 | 17.344 | 1.00 | 0.00 | 3A4 |
| ATOM | 281 | O   | THR | 84 | 14.500 | 19.282 | 16.144 | 1.00 | 0.00 | 3A4 |
| ATOM | 282 | N   | ASP | 85 | 14.371 | 20.231 | 18.176 | 1.00 | 0.00 | 3A4 |
| ATOM | 283 | CA  | ASP | 85 | 14.595 | 21.594 | 17.732 | 1.00 | 0.00 | 3A4 |
| ATOM | 284 | CB  | ASP | 85 | 13.703 | 22.550 | 18.577 | 1.00 | 0.00 | 3A4 |
| ATOM | 285 | CG  | ASP | 85 | 13.371 | 23.873 | 17.872 | 1.00 | 0.00 | 3A4 |
| ATOM | 286 | OD1 | ASP | 85 | 12.666 | 23.828 | 16.828 | 1.00 | 0.00 | 3A4 |
| ATOM | 287 | OD2 | ASP | 85 | 13.808 | 24.942 | 18.373 | 1.00 | 0.00 | 3A4 |
| ATOM | 288 | C   | ASP | 85 | 16.050 | 21.928 | 17.888 | 1.00 | 0.00 | 3A4 |
| ATOM | 289 | O   | ASP | 85 | 16.660 | 21.452 | 18.843 | 1.00 | 0.00 | 3A4 |
| ATOM | 290 | N   | PRO | 86 | 16.683 | 22.732 | 17.024 | 1.00 | 0.00 | 3A4 |
| ATOM | 291 | CA  | PRO | 86 | 18.101 | 23.035 | 17.076 | 1.00 | 0.00 | 3A4 |
| ATOM | 292 | CD  | PRO | 86 | 16.102 | 23.257 | 15.807 | 1.00 | 0.00 | 3A4 |
| ATOM | 293 | CB  | PRO | 86 | 18.421 | 23.751 | 15.747 | 1.00 | 0.00 | 3A4 |
| ATOM | 294 | CG  | PRO | 86 | 17.079 | 24.309 | 15.294 | 1.00 | 0.00 | 3A4 |
| ATOM | 295 | C   | PRO | 86 | 18.425 | 23.863 | 18.284 | 1.00 | 0.00 | 3A4 |
| ATOM | 296 | O   | PRO | 86 | 19.466 | 23.647 | 18.892 | 1.00 | 0.00 | 3A4 |
| ATOM | 297 | N   | ASP | 87 | 17.511 | 24.756 | 18.711 | 1.00 | 0.00 | 3A4 |
| ATOM | 298 | CA  | ASP | 87 | 17.636 | 25.559 | 19.902 | 1.00 | 0.00 | 3A4 |
| ATOM | 299 | CB  | ASP | 87 | 16.417 | 26.494 | 20.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 300 | CG  | ASP | 87 | 16.305 | 27.442 | 18.820 | 1.00 | 0.00 | 3A4 |
| ATOM | 301 | OD1 | ASP | 87 | 17.357 | 27.851 | 18.258 | 1.00 | 0.00 | 3A4 |
| ATOM | 302 | OD2 | ASP | 87 | 15.148 | 27.764 | 18.439 | 1.00 | 0.00 | 3A4 |
| ATOM | 303 | C   | ASP | 87 | 17.724 | 24.745 | 21.171 | 1.00 | 0.00 | 3A4 |
| ATOM | 304 | O   | ASP | 87 | 18.546 | 25.018 | 22.032 | 1.00 | 0.00 | 3A4 |
| ATOM | 305 | N   | MET | 88 | 16.902 | 23.678 | 21.253 | 1.00 | 0.00 | 3A4 |
| ATOM | 306 | CA  | MET | 88 | 16.847 | 22.776 | 22.375 | 1.00 | 0.00 | 3A4 |
| ATOM | 307 | CB  | MET | 88 | 15.536 | 22.000 | 22.396 | 1.00 | 0.00 | 3A4 |
| ATOM | 308 | CG  | MET | 88 | 14.362 | 22.948 | 22.644 | 1.00 | 0.00 | 3A4 |
| ATOM | 309 | SD  | MET | 88 | 12.947 | 22.177 | 23.469 | 1.00 | 0.00 | 3A4 |
| ATOM | 310 | CE  | MET | 88 | 13.722 | 21.914 | 25.087 | 1.00 | 0.00 | 3A4 |
| ATOM | 311 | C   | MET | 88 | 18.007 | 21.812 | 22.436 | 1.00 | 0.00 | 3A4 |
| ATOM | 312 | O   | MET | 88 | 18.524 | 21.506 | 23.506 | 1.00 | 0.00 | 3A4 |
| ATOM | 313 | N   | ILE | 89 | 18.500 | 21.349 | 21.264 | 1.00 | 0.00 | 3A4 |
| ATOM | 314 | CA  | ILE | 89 | 19.637 | 20.450 | 21.170 | 1.00 | 0.00 | 3A4 |
| ATOM | 315 | CB  | ILE | 89 | 19.679 | 19.800 | 19.793 | 1.00 | 0.00 | 3A4 |
| ATOM | 316 | CG2 | ILE | 89 | 21.088 | 19.217 | 19.442 | 1.00 | 0.00 | 3A4 |
| ATOM | 317 | CG1 | ILE | 89 | 18.596 | 18.681 | 19.910 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |    |        |        |        |      |      |     |
|------|-----|-----|-----|----|--------|--------|--------|------|------|-----|
| ATOM | 318 | CD  | ILE | 89 | 18.390 | 17.678 | 18.773 | 1.00 | 0.00 | 3A4 |
| ATOM | 319 | C   | ILE | 89 | 20.916 | 21.161 | 21.538 | 1.00 | 0.00 | 3A4 |
| ATOM | 320 | O   | ILE | 89 | 21.722 | 20.655 | 22.310 | 1.00 | 0.00 | 3A4 |
| ATOM | 321 | N   | LYS | 90 | 21.096 | 22.421 | 21.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 322 | CA  | LYS | 90 | 22.214 | 23.250 | 21.481 | 1.00 | 0.00 | 3A4 |
| ATOM | 323 | CB  | LYS | 90 | 22.225 | 24.577 | 20.719 | 1.00 | 0.00 | 3A4 |
| ATOM | 324 | CG  | LYS | 90 | 23.531 | 25.387 | 20.790 | 1.00 | 0.00 | 3A4 |
| ATOM | 325 | CD  | LYS | 90 | 23.546 | 26.569 | 19.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 326 | CE  | LYS | 90 | 24.875 | 27.339 | 19.774 | 1.00 | 0.00 | 3A4 |
| ATOM | 327 | NZ  | LYS | 90 | 25.167 | 27.975 | 21.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 328 | C   | LYS | 90 | 22.221 | 23.564 | 22.961 | 1.00 | 0.00 | 3A4 |
| ATOM | 329 | O   | LYS | 90 | 23.248 | 23.567 | 23.612 | 1.00 | 0.00 | 3A4 |
| ATOM | 330 | N   | THR | 91 | 21.031 | 23.752 | 23.561 | 1.00 | 0.00 | 3A4 |
| ATOM | 331 | CA  | THR | 91 | 20.855 | 23.981 | 24.981 | 1.00 | 0.00 | 3A4 |
| ATOM | 332 | CB  | THR | 91 | 19.434 | 24.380 | 25.293 | 1.00 | 0.00 | 3A4 |
| ATOM | 333 | OG1 | THR | 91 | 19.170 | 25.637 | 24.681 | 1.00 | 0.00 | 3A4 |
| ATOM | 334 | CG2 | THR | 91 | 19.109 | 24.554 | 26.810 | 1.00 | 0.00 | 3A4 |
| ATOM | 335 | C   | THR | 91 | 21.198 | 22.782 | 25.817 | 1.00 | 0.00 | 3A4 |
| ATOM | 336 | O   | THR | 91 | 21.850 | 22.889 | 26.851 | 1.00 | 0.00 | 3A4 |
| ATOM | 337 | N   | VAL | 92 | 20.849 | 21.578 | 25.307 | 1.00 | 0.00 | 3A4 |
| ATOM | 338 | CA  | VAL | 92 | 21.125 | 20.315 | 25.945 | 1.00 | 0.00 | 3A4 |
| ATOM | 339 | CB  | VAL | 92 | 20.299 | 19.178 | 25.353 | 1.00 | 0.00 | 3A4 |
| ATOM | 340 | CG1 | VAL | 92 | 21.025 | 18.247 | 24.370 | 1.00 | 0.00 | 3A4 |
| ATOM | 341 | CG2 | VAL | 92 | 19.643 | 18.370 | 26.498 | 1.00 | 0.00 | 3A4 |
| ATOM | 342 | C   | VAL | 92 | 22.600 | 20.047 | 26.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 343 | O   | VAL | 92 | 22.991 | 19.412 | 27.041 | 1.00 | 0.00 | 3A4 |
| ATOM | 344 | N   | LEU | 93 | 23.483 | 20.706 | 25.311 | 1.00 | 0.00 | 3A4 |
| ATOM | 345 | CA  | LEU | 93 | 24.914 | 20.851 | 25.543 | 1.00 | 0.00 | 3A4 |
| ATOM | 346 | CB  | LEU | 93 | 25.432 | 21.742 | 24.407 | 1.00 | 0.00 | 3A4 |
| ATOM | 347 | CG  | LEU | 93 | 26.456 | 21.108 | 23.525 | 1.00 | 0.00 | 3A4 |
| ATOM | 348 | CD1 | LEU | 93 | 25.796 | 19.892 | 22.820 | 1.00 | 0.00 | 3A4 |
| ATOM | 349 | CD2 | LEU | 93 | 26.955 | 22.238 | 22.601 | 1.00 | 0.00 | 3A4 |
| ATOM | 350 | C   | LEU | 93 | 25.419 | 21.473 | 26.847 | 1.00 | 0.00 | 3A4 |
| ATOM | 351 | O   | LEU | 93 | 24.654 | 21.997 | 27.655 | 1.00 | 0.00 | 3A4 |
| ATOM | 352 | N   | VAL | 94 | 26.774 | 21.385 | 27.035 | 1.00 | 0.00 | 3A4 |
| ATOM | 353 | CA  | VAL | 94 | 27.599 | 21.729 | 28.196 | 1.00 | 0.00 | 3A4 |
| ATOM | 354 | CB  | VAL | 94 | 27.328 | 23.082 | 28.879 | 1.00 | 0.00 | 3A4 |
| ATOM | 355 | CG1 | VAL | 94 | 28.368 | 23.358 | 30.001 | 1.00 | 0.00 | 3A4 |
| ATOM | 356 | CG2 | VAL | 94 | 27.427 | 24.201 | 27.813 | 1.00 | 0.00 | 3A4 |
| ATOM | 357 | C   | VAL | 94 | 27.515 | 20.540 | 29.137 | 1.00 | 0.00 | 3A4 |
| ATOM | 358 | O   | VAL | 94 | 26.875 | 20.578 | 30.188 | 1.00 | 0.00 | 3A4 |
| ATOM | 359 | N   | LYS | 95 | 28.141 | 19.421 | 28.690 | 1.00 | 0.00 | 3A4 |
| ATOM | 360 | CA  | LYS | 95 | 28.019 | 18.101 | 29.261 | 1.00 | 0.00 | 3A4 |
| ATOM | 361 | CB  | LYS | 95 | 27.404 | 17.078 | 28.259 | 1.00 | 0.00 | 3A4 |
| ATOM | 362 | CG  | LYS | 95 | 27.757 | 17.284 | 26.778 | 1.00 | 0.00 | 3A4 |
| ATOM | 363 | CD  | LYS | 95 | 27.133 | 16.199 | 25.898 | 1.00 | 0.00 | 3A4 |
| ATOM | 364 | CE  | LYS | 95 | 27.017 | 16.559 | 24.413 | 1.00 | 0.00 | 3A4 |
| ATOM | 365 | NZ  | LYS | 95 | 28.338 | 16.819 | 23.809 | 1.00 | 0.00 | 3A4 |
| ATOM | 366 | C   | LYS | 95 | 29.379 | 17.675 | 29.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 367 | O   | LYS | 95 | 30.123 | 16.990 | 29.040 | 1.00 | 0.00 | 3A4 |
| ATOM | 368 | N   | GLU | 96 | 29.703 | 18.085 | 30.988 | 1.00 | 0.00 | 3A4 |
| ATOM | 369 | CA  | GLU | 96 | 30.926 | 17.783 | 31.698 | 1.00 | 0.00 | 3A4 |
| ATOM | 370 | CB  | GLU | 96 | 31.795 | 19.051 | 31.950 | 1.00 | 0.00 | 3A4 |
| ATOM | 371 | CG  | GLU | 96 | 31.039 | 20.290 | 32.486 | 1.00 | 0.00 | 3A4 |
| ATOM | 372 | CD  | GLU | 96 | 32.012 | 21.467 | 32.599 | 1.00 | 0.00 | 3A4 |
| ATOM | 373 | OE1 | GLU | 96 | 31.790 | 22.493 | 31.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 374 | OE2 | GLU | 96 | 32.990 | 21.357 | 33.388 | 1.00 | 0.00 | 3A4 |
| ATOM | 375 | C   | GLU | 96 | 30.517 | 17.078 | 32.969 | 1.00 | 0.00 | 3A4 |
| ATOM | 376 | O   | GLU | 96 | 30.732 | 17.576 | 34.073 | 1.00 | 0.00 | 3A4 |
| ATOM | 377 | N   | CYS | 97 | 29.924 | 15.869 | 32.763 | 1.00 | 0.00 | 3A4 |
| ATOM | 378 | CA  | CYS | 97 | 29.436 | 14.865 | 33.693 | 1.00 | 0.00 | 3A4 |
| ATOM | 379 | CB  | CYS | 97 | 29.558 | 15.141 | 35.235 | 1.00 | 0.00 | 3A4 |
| ATOM | 380 | SG  | CYS | 97 | 29.186 | 13.706 | 36.313 | 1.00 | 0.00 | 3A4 |
| ATOM | 381 | C   | CYS | 97 | 28.000 | 14.633 | 33.277 | 1.00 | 0.00 | 3A4 |
| ATOM | 382 | O   | CYS | 97 | 27.076 | 15.253 | 33.800 | 1.00 | 0.00 | 3A4 |
| ATOM | 383 | N   | TYR | 98 | 27.817 | 13.703 | 32.305 | 1.00 | 0.00 | 3A4 |
| ATOM | 384 | CA  | TYR | 98 | 26.556 | 13.216 | 31.782 | 1.00 | 0.00 | 3A4 |
| ATOM | 385 | CB  | TYR | 98 | 26.197 | 13.814 | 30.380 | 1.00 | 0.00 | 3A4 |
| ATOM | 386 | CG  | TYR | 98 | 25.205 | 14.939 | 30.543 | 1.00 | 0.00 | 3A4 |
| ATOM | 387 | CD1 | TYR | 98 | 25.573 | 16.198 | 31.050 | 1.00 | 0.00 | 3A4 |
| ATOM | 388 | CD2 | TYR | 98 | 23.862 | 14.731 | 30.197 | 1.00 | 0.00 | 3A4 |
| ATOM | 389 | CE1 | TYR | 98 | 24.626 | 17.224 | 31.198 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |        |      |      |     |
|------|-----|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 390 | CE2 | TYR | 98  | 22.901 | 15.740 | 30.351 | 1.00 | 0.00 | 3A4 |
| ATOM | 391 | CZ  | TYR | 98  | 23.286 | 16.993 | 30.849 | 1.00 | 0.00 | 3A4 |
| ATOM | 392 | OH  | TYR | 98  | 22.323 | 18.015 | 30.999 | 1.00 | 0.00 | 3A4 |
| ATOM | 393 | C   | TYR | 98  | 26.800 | 11.735 | 31.683 | 1.00 | 0.00 | 3A4 |
| ATOM | 394 | O   | TYR | 98  | 27.629 | 11.292 | 30.891 | 1.00 | 0.00 | 3A4 |
| ATOM | 395 | N   | SER | 99  | 26.097 | 10.928 | 32.531 | 1.00 | 0.00 | 3A4 |
| ATOM | 396 | CA  | SER | 99  | 26.414 | 9.536  | 32.838 | 1.00 | 0.00 | 3A4 |
| ATOM | 397 | CB  | SER | 99  | 25.870 | 9.141  | 34.247 | 1.00 | 0.00 | 3A4 |
| ATOM | 398 | OG  | SER | 99  | 26.515 | 7.992  | 34.791 | 1.00 | 0.00 | 3A4 |
| ATOM | 399 | C   | SER | 99  | 25.931 | 8.568  | 31.771 | 1.00 | 0.00 | 3A4 |
| ATOM | 400 | O   | SER | 99  | 24.885 | 8.764  | 31.156 | 1.00 | 0.00 | 3A4 |
| ATOM | 401 | N   | VAL | 100 | 26.759 | 7.507  | 31.524 | 1.00 | 0.00 | 3A4 |
| ATOM | 402 | CA  | VAL | 100 | 26.647 | 6.426  | 30.542 | 1.00 | 0.00 | 3A4 |
| ATOM | 403 | CB  | VAL | 100 | 25.344 | 5.612  | 30.576 | 1.00 | 0.00 | 3A4 |
| ATOM | 404 | CG1 | VAL | 100 | 25.483 | 4.356  | 29.677 | 1.00 | 0.00 | 3A4 |
| ATOM | 405 | CG2 | VAL | 100 | 25.062 | 5.167  | 32.031 | 1.00 | 0.00 | 3A4 |
| ATOM | 406 | C   | VAL | 100 | 26.977 | 6.962  | 29.152 | 1.00 | 0.00 | 3A4 |
| ATOM | 407 | O   | VAL | 100 | 28.088 | 6.758  | 28.673 | 1.00 | 0.00 | 3A4 |
| ATOM | 408 | N   | PHE | 101 | 26.002 | 7.682  | 28.517 | 1.00 | 0.00 | 3A4 |
| ATOM | 409 | CA  | PHE | 101 | 26.131 | 8.581  | 27.372 | 1.00 | 0.00 | 3A4 |
| ATOM | 410 | CB  | PHE | 101 | 27.487 | 9.383  | 27.359 | 1.00 | 0.00 | 3A4 |
| ATOM | 411 | CG  | PHE | 101 | 27.503 | 10.546 | 26.402 | 1.00 | 0.00 | 3A4 |
| ATOM | 412 | CD1 | PHE | 101 | 26.587 | 11.609 | 26.522 | 1.00 | 0.00 | 3A4 |
| ATOM | 413 | CD2 | PHE | 101 | 28.432 | 10.563 | 25.350 | 1.00 | 0.00 | 3A4 |
| ATOM | 414 | CE1 | PHE | 101 | 26.580 | 12.640 | 25.573 | 1.00 | 0.00 | 3A4 |
| ATOM | 415 | CE2 | PHE | 101 | 28.435 | 11.597 | 24.418 | 1.00 | 0.00 | 3A4 |
| ATOM | 416 | CZ  | PHE | 101 | 27.492 | 12.629 | 24.516 | 1.00 | 0.00 | 3A4 |
| ATOM | 417 | C   | PHE | 101 | 25.860 | 7.863  | 26.049 | 1.00 | 0.00 | 3A4 |
| ATOM | 418 | O   | PHE | 101 | 25.613 | 8.506  | 25.030 | 1.00 | 0.00 | 3A4 |
| ATOM | 419 | N   | THR | 102 | 25.881 | 6.507  | 26.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 420 | CA  | THR | 102 | 25.468 | 5.674  | 24.939 | 1.00 | 0.00 | 3A4 |
| ATOM | 421 | CB  | THR | 102 | 26.561 | 5.456  | 23.875 | 1.00 | 0.00 | 3A4 |
| ATOM | 422 | OG1 | THR | 102 | 26.134 | 4.618  | 22.803 | 1.00 | 0.00 | 3A4 |
| ATOM | 423 | CG2 | THR | 102 | 27.920 | 4.971  | 24.441 | 1.00 | 0.00 | 3A4 |
| ATOM | 424 | C   | THR | 102 | 24.949 | 4.448  | 25.660 | 1.00 | 0.00 | 3A4 |
| ATOM | 425 | O   | THR | 102 | 25.680 | 3.511  | 25.976 | 1.00 | 0.00 | 3A4 |
| ATOM | 426 | N   | ASN | 103 | 23.629 | 4.491  | 25.991 | 1.00 | 0.00 | 3A4 |
| ATOM | 427 | CA  | ASN | 103 | 22.973 | 3.634  | 26.965 | 1.00 | 0.00 | 3A4 |
| ATOM | 428 | CB  | ASN | 103 | 22.145 | 4.482  | 28.000 | 1.00 | 0.00 | 3A4 |
| ATOM | 429 | CG  | ASN | 103 | 21.193 | 5.519  | 27.373 | 1.00 | 0.00 | 3A4 |
| ATOM | 430 | OD1 | ASN | 103 | 21.530 | 6.702  | 27.345 | 1.00 | 0.00 | 3A4 |
| ATOM | 431 | ND2 | ASN | 103 | 19.993 | 5.093  | 26.893 | 1.00 | 0.00 | 3A4 |
| ATOM | 432 | C   | ASN | 103 | 22.171 | 2.529  | 26.295 | 1.00 | 0.00 | 3A4 |
| ATOM | 433 | O   | ASN | 103 | 22.526 | 2.061  | 25.214 | 1.00 | 0.00 | 3A4 |
| ATOM | 434 | N   | ARG | 104 | 21.099 | 2.084  | 27.018 | 1.00 | 0.00 | 3A4 |
| ATOM | 435 | CA  | ARG | 104 | 20.255 | 0.904  | 26.922 | 1.00 | 0.00 | 3A4 |
| ATOM | 436 | CB  | ARG | 104 | 20.057 | 0.305  | 25.521 | 1.00 | 0.00 | 3A4 |
| ATOM | 437 | CG  | ARG | 104 | 19.266 | 1.224  | 24.571 | 1.00 | 0.00 | 3A4 |
| ATOM | 438 | CD  | ARG | 104 | 19.318 | 0.794  | 23.096 | 1.00 | 0.00 | 3A4 |
| ATOM | 439 | NE  | ARG | 104 | 20.722 | 1.001  | 22.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 440 | CZ  | ARG | 104 | 21.086 | 0.812  | 21.280 | 1.00 | 0.00 | 3A4 |
| ATOM | 441 | NH1 | ARG | 104 | 22.383 | 1.027  | 20.912 | 1.00 | 0.00 | 3A4 |
| ATOM | 442 | NH2 | ARG | 104 | 20.184 | 0.403  | 20.340 | 1.00 | 0.00 | 3A4 |
| ATOM | 443 | C   | ARG | 104 | 20.801 | -0.116 | 27.892 | 1.00 | 0.00 | 3A4 |
| ATOM | 444 | O   | ARG | 104 | 21.996 | -0.173 | 28.177 | 1.00 | 0.00 | 3A4 |
| ATOM | 445 | N   | ARG | 105 | 19.899 | -0.953 | 28.439 | 1.00 | 0.00 | 3A4 |
| ATOM | 446 | CA  | ARG | 105 | 20.180 | -1.924 | 29.470 | 1.00 | 0.00 | 3A4 |
| ATOM | 447 | CB  | ARG | 105 | 18.917 | -2.306 | 30.269 | 1.00 | 0.00 | 3A4 |
| ATOM | 448 | CG  | ARG | 105 | 18.288 | -1.109 | 31.012 | 1.00 | 0.00 | 3A4 |
| ATOM | 449 | CD  | ARG | 105 | 17.273 | -0.267 | 30.201 | 1.00 | 0.00 | 3A4 |
| ATOM | 450 | NE  | ARG | 105 | 16.999 | 1.019  | 30.940 | 1.00 | 0.00 | 3A4 |
| ATOM | 451 | CZ  | ARG | 105 | 17.736 | 2.168  | 30.769 | 1.00 | 0.00 | 3A4 |
| ATOM | 452 | NH1 | ARG | 105 | 17.471 | 3.253  | 31.550 | 1.00 | 0.00 | 3A4 |
| ATOM | 453 | NH2 | ARG | 105 | 18.734 | 2.262  | 29.841 | 1.00 | 0.00 | 3A4 |
| ATOM | 454 | C   | ARG | 105 | 20.851 | -3.183 | 28.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 455 | O   | ARG | 105 | 21.862 | -3.545 | 29.576 | 1.00 | 0.00 | 3A4 |
| ATOM | 456 | N   | PRO | 106 | 20.439 | -3.879 | 27.908 | 1.00 | 0.00 | 3A4 |
| ATOM | 457 | CA  | PRO | 106 | 21.118 | -5.066 | 27.409 | 1.00 | 0.00 | 3A4 |
| ATOM | 458 | CD  | PRO | 106 | 19.166 | -3.707 | 27.212 | 1.00 | 0.00 | 3A4 |
| ATOM | 459 | CB  | PRO | 106 | 20.292 | -5.535 | 26.208 | 1.00 | 0.00 | 3A4 |
| ATOM | 460 | CG  | PRO | 106 | 19.354 | -4.383 | 25.861 | 1.00 | 0.00 | 3A4 |
| ATOM | 461 | C   | PRO | 106 | 22.531 | -4.785 | 26.960 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |        |      |      |     |
|------|-----|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 462 | O   | PRO | 106 | 23.412 | -5.580 | 27.239 | 1.00 | 0.00 | 3A4 |
| ATOM | 463 | N   | PHE | 107 | 22.789 | -3.612 | 26.347 | 1.00 | 0.00 | 3A4 |
| ATOM | 464 | CA  | PHE | 107 | 24.092 | -3.149 | 25.939 | 1.00 | 0.00 | 3A4 |
| ATOM | 465 | CB  | PHE | 107 | 23.996 | -1.854 | 25.067 | 1.00 | 0.00 | 3A4 |
| ATOM | 466 | CG  | PHE | 107 | 23.377 | -2.185 | 23.730 | 1.00 | 0.00 | 3A4 |
| ATOM | 467 | CD1 | PHE | 107 | 24.194 | -2.404 | 22.604 | 1.00 | 0.00 | 3A4 |
| ATOM | 468 | CD2 | PHE | 107 | 21.982 | -2.301 | 23.578 | 1.00 | 0.00 | 3A4 |
| ATOM | 469 | CE1 | PHE | 107 | 23.633 | -2.730 | 21.360 | 1.00 | 0.00 | 3A4 |
| ATOM | 470 | CE2 | PHE | 107 | 21.415 | -2.640 | 22.342 | 1.00 | 0.00 | 3A4 |
| ATOM | 471 | CZ  | PHE | 107 | 22.243 | -2.850 | 21.231 | 1.00 | 0.00 | 3A4 |
| ATOM | 472 | C   | PHE | 107 | 24.996 | -2.874 | 27.117 | 1.00 | 0.00 | 3A4 |
| ATOM | 473 | O   | PHE | 107 | 26.183 | -3.178 | 27.071 | 1.00 | 0.00 | 3A4 |
| ATOM | 474 | N   | GLY | 108 | 24.445 | -2.352 | 28.235 | 1.00 | 0.00 | 3A4 |
| ATOM | 475 | CA  | GLY | 108 | 25.169 | -2.115 | 29.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 476 | C   | GLY | 108 | 25.703 | -3.372 | 30.122 | 1.00 | 0.00 | 3A4 |
| ATOM | 477 | O   | GLY | 108 | 26.825 | -3.365 | 30.623 | 1.00 | 0.00 | 3A4 |
| ATOM | 478 | N   | PRO | 109 | 24.957 | -4.476 | 30.112 | 1.00 | 0.00 | 3A4 |
| ATOM | 479 | CA  | PRO | 109 | 25.476 | -5.825 | 30.348 | 1.00 | 0.00 | 3A4 |
| ATOM | 480 | CD  | PRO | 109 | 24.065 | -4.305 | 31.286 | 1.00 | 0.00 | 3A4 |
| ATOM | 481 | CB  | PRO | 109 | 24.191 | -6.637 | 30.615 | 1.00 | 0.00 | 3A4 |
| ATOM | 482 | CG  | PRO | 109 | 23.330 | -5.658 | 31.433 | 1.00 | 0.00 | 3A4 |
| ATOM | 483 | C   | PRO | 109 | 26.330 | -6.541 | 29.318 | 1.00 | 0.00 | 3A4 |
| ATOM | 484 | O   | PRO | 109 | 27.456 | -6.908 | 29.658 | 1.00 | 0.00 | 3A4 |
| ATOM | 485 | N   | VAL | 110 | 25.774 | -6.864 | 28.119 | 1.00 | 0.00 | 3A4 |
| ATOM | 486 | CA  | VAL | 110 | 26.331 | -7.778 | 27.133 | 1.00 | 0.00 | 3A4 |
| ATOM | 487 | CB  | VAL | 110 | 25.389 | -8.936 | 26.768 | 1.00 | 0.00 | 3A4 |
| ATOM | 488 | CG1 | VAL | 110 | 25.412 | -9.943 | 27.938 | 1.00 | 0.00 | 3A4 |
| ATOM | 489 | CG2 | VAL | 110 | 23.943 | -8.492 | 26.450 | 1.00 | 0.00 | 3A4 |
| ATOM | 490 | C   | VAL | 110 | 26.744 | -6.971 | 25.923 | 1.00 | 0.00 | 3A4 |
| ATOM | 491 | O   | VAL | 110 | 25.981 | -6.165 | 25.392 | 1.00 | 0.00 | 3A4 |
| ATOM | 492 | N   | GLY | 111 | 28.021 | -7.174 | 25.497 | 1.00 | 0.00 | 3A4 |
| ATOM | 493 | CA  | GLY | 111 | 28.732 | -6.403 | 24.496 | 1.00 | 0.00 | 3A4 |
| ATOM | 494 | C   | GLY | 111 | 29.773 | -5.622 | 25.245 | 1.00 | 0.00 | 3A4 |
| ATOM | 495 | O   | GLY | 111 | 29.468 | -4.588 | 25.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 496 | N   | PHE | 112 | 31.035 | -6.136 | 25.266 | 1.00 | 0.00 | 3A4 |
| ATOM | 497 | CA  | PHE | 112 | 32.105 | -5.711 | 26.158 | 1.00 | 0.00 | 3A4 |
| ATOM | 498 | CB  | PHE | 112 | 32.907 | -6.929 | 26.720 | 1.00 | 0.00 | 3A4 |
| ATOM | 499 | CG  | PHE | 112 | 31.979 | -7.800 | 27.529 | 1.00 | 0.00 | 3A4 |
| ATOM | 500 | CD1 | PHE | 112 | 31.631 | -9.095 | 27.096 | 1.00 | 0.00 | 3A4 |
| ATOM | 501 | CD2 | PHE | 112 | 31.424 | -7.318 | 28.732 | 1.00 | 0.00 | 3A4 |
| ATOM | 502 | CE1 | PHE | 112 | 30.746 | -9.883 | 27.847 | 1.00 | 0.00 | 3A4 |
| ATOM | 503 | CE2 | PHE | 112 | 30.537 | -8.104 | 29.480 | 1.00 | 0.00 | 3A4 |
| ATOM | 504 | CZ  | PHE | 112 | 30.195 | -9.387 | 29.035 | 1.00 | 0.00 | 3A4 |
| ATOM | 505 | C   | PHE | 112 | 33.050 | -4.749 | 25.472 | 1.00 | 0.00 | 3A4 |
| ATOM | 506 | O   | PHE | 112 | 34.190 | -5.078 | 25.148 | 1.00 | 0.00 | 3A4 |
| ATOM | 507 | N   | MET | 113 | 32.562 | -3.489 | 25.295 | 1.00 | 0.00 | 3A4 |
| ATOM | 508 | CA  | MET | 113 | 33.296 | -2.314 | 24.869 | 1.00 | 0.00 | 3A4 |
| ATOM | 509 | CB  | MET | 113 | 32.602 | -1.505 | 23.728 | 1.00 | 0.00 | 3A4 |
| ATOM | 510 | CG  | MET | 113 | 32.554 | -2.210 | 22.356 | 1.00 | 0.00 | 3A4 |
| ATOM | 511 | SD  | MET | 113 | 31.429 | -3.639 | 22.184 | 1.00 | 0.00 | 3A4 |
| ATOM | 512 | CE  | MET | 113 | 29.851 | -2.787 | 22.471 | 1.00 | 0.00 | 3A4 |
| ATOM | 513 | C   | MET | 113 | 33.386 | -1.481 | 26.125 | 1.00 | 0.00 | 3A4 |
| ATOM | 514 | O   | MET | 113 | 32.371 | -1.027 | 26.652 | 1.00 | 0.00 | 3A4 |
| ATOM | 515 | N   | LYS | 114 | 34.630 | -1.321 | 26.660 | 1.00 | 0.00 | 3A4 |
| ATOM | 516 | CA  | LYS | 114 | 34.932 | -0.910 | 28.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 517 | CB  | LYS | 114 | 36.207 | -1.643 | 28.544 | 1.00 | 0.00 | 3A4 |
| ATOM | 518 | CG  | LYS | 114 | 36.129 | -3.170 | 28.392 | 1.00 | 0.00 | 3A4 |
| ATOM | 519 | CD  | LYS | 114 | 37.411 | -3.890 | 28.832 | 1.00 | 0.00 | 3A4 |
| ATOM | 520 | CE  | LYS | 114 | 37.355 | -5.417 | 28.667 | 1.00 | 0.00 | 3A4 |
| ATOM | 521 | NZ  | LYS | 114 | 37.190 | -5.806 | 27.244 | 1.00 | 0.00 | 3A4 |
| ATOM | 522 | C   | LYS | 114 | 35.074 | 0.600  | 28.136 | 1.00 | 0.00 | 3A4 |
| ATOM | 523 | O   | LYS | 114 | 34.485 | 1.339  | 27.348 | 1.00 | 0.00 | 3A4 |
| ATOM | 524 | N   | SER | 115 | 35.857 | 1.092  | 29.141 | 1.00 | 0.00 | 3A4 |
| ATOM | 525 | CA  | SER | 115 | 35.955 | 2.486  | 29.566 | 1.00 | 0.00 | 3A4 |
| ATOM | 526 | CB  | SER | 115 | 36.419 | 2.597  | 31.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 527 | OG  | SER | 115 | 35.505 | 1.921  | 31.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 528 | C   | SER | 115 | 36.891 | 3.307  | 28.696 | 1.00 | 0.00 | 3A4 |
| ATOM | 529 | O   | SER | 115 | 38.106 | 3.302  | 28.890 | 1.00 | 0.00 | 3A4 |
| ATOM | 530 | N   | ALA | 116 | 36.300 | 4.041  | 27.709 | 1.00 | 0.00 | 3A4 |
| ATOM | 531 | CA  | ALA | 116 | 36.990 | 4.902  | 26.770 | 1.00 | 0.00 | 3A4 |
| ATOM | 532 | CB  | ALA | 116 | 36.806 | 4.440  | 25.323 | 1.00 | 0.00 | 3A4 |
| ATOM | 533 | C   | ALA | 116 | 36.445 | 6.277  | 26.942 | 1.00 | 0.00 | 3A4 |



|      |     |     |     |     |        |        |        |      |      |     |
|------|-----|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 534 | O   | ALA | 116 | 35.934 | 6.634  | 27.995 | 1.00 | 0.00 | 3A4 |
| ATOM | 535 | N   | ILE | 117 | 36.498 | 7.116  | 25.886 | 1.00 | 0.00 | 3A4 |
| ATOM | 536 | CA  | ILE | 117 | 36.054 | 8.497  | 25.985 | 1.00 | 0.00 | 3A4 |
| ATOM | 537 | CB  | ILE | 117 | 36.818 | 9.363  | 24.999 | 1.00 | 0.00 | 3A4 |
| ATOM | 538 | CG2 | ILE | 117 | 36.637 | 8.922  | 23.524 | 1.00 | 0.00 | 3A4 |
| ATOM | 539 | CG1 | ILE | 117 | 36.647 | 10.857 | 25.212 | 1.00 | 0.00 | 3A4 |
| ATOM | 540 | CD  | ILE | 117 | 37.122 | 11.262 | 26.574 | 1.00 | 0.00 | 3A4 |
| ATOM | 541 | C   | ILE | 117 | 34.556 | 8.659  | 25.822 | 1.00 | 0.00 | 3A4 |
| ATOM | 542 | O   | ILE | 117 | 33.924 | 9.474  | 26.492 | 1.00 | 0.00 | 3A4 |
| ATOM | 543 | N   | SER | 118 | 33.923 | 7.843  | 24.946 | 1.00 | 0.00 | 3A4 |
| ATOM | 544 | CA  | SER | 118 | 32.533 | 8.033  | 24.588 | 1.00 | 0.00 | 3A4 |
| ATOM | 545 | CB  | SER | 118 | 32.205 | 7.525  | 23.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 546 | OG  | SER | 118 | 32.499 | 6.147  | 22.946 | 1.00 | 0.00 | 3A4 |
| ATOM | 547 | C   | SER | 118 | 31.585 | 7.455  | 25.606 | 1.00 | 0.00 | 3A4 |
| ATOM | 548 | O   | SER | 118 | 30.395 | 7.686  | 25.524 | 1.00 | 0.00 | 3A4 |
| ATOM | 549 | N   | ILE | 119 | 32.084 | 6.735  | 26.630 | 1.00 | 0.00 | 3A4 |
| ATOM | 550 | CA  | ILE | 119 | 31.251 | 6.157  | 27.657 | 1.00 | 0.00 | 3A4 |
| ATOM | 551 | CB  | ILE | 119 | 31.480 | 4.637  | 27.705 | 1.00 | 0.00 | 3A4 |
| ATOM | 552 | CG2 | ILE | 119 | 32.895 | 4.296  | 28.225 | 1.00 | 0.00 | 3A4 |
| ATOM | 553 | CG1 | ILE | 119 | 30.373 | 3.794  | 28.400 | 1.00 | 0.00 | 3A4 |
| ATOM | 554 | CD  | ILE | 119 | 29.071 | 3.681  | 27.605 | 1.00 | 0.00 | 3A4 |
| ATOM | 555 | C   | ILE | 119 | 31.475 | 6.827  | 29.005 | 1.00 | 0.00 | 3A4 |
| ATOM | 556 | O   | ILE | 119 | 30.894 | 6.426  | 30.013 | 1.00 | 0.00 | 3A4 |
| ATOM | 557 | N   | ALA | 120 | 32.350 | 7.862  | 29.050 | 1.00 | 0.00 | 3A4 |
| ATOM | 558 | CA  | ALA | 120 | 32.876 | 8.420  | 30.276 | 1.00 | 0.00 | 3A4 |
| ATOM | 559 | CB  | ALA | 120 | 34.429 | 8.417  | 30.275 | 1.00 | 0.00 | 3A4 |
| ATOM | 560 | C   | ALA | 120 | 32.403 | 9.821  | 30.537 | 1.00 | 0.00 | 3A4 |
| ATOM | 561 | O   | ALA | 120 | 32.153 | 10.624 | 29.642 | 1.00 | 0.00 | 3A4 |
| ATOM | 562 | N   | GLU | 121 | 32.338 | 10.132 | 31.847 | 1.00 | 0.00 | 3A4 |
| ATOM | 563 | CA  | GLU | 121 | 31.987 | 11.402 | 32.421 | 1.00 | 0.00 | 3A4 |
| ATOM | 564 | CB  | GLU | 121 | 31.189 | 11.213 | 33.742 | 1.00 | 0.00 | 3A4 |
| ATOM | 565 | CG  | GLU | 121 | 29.884 | 10.420 | 33.613 | 1.00 | 0.00 | 3A4 |
| ATOM | 566 | CD  | GLU | 121 | 30.124 | 8.902  | 33.618 | 1.00 | 0.00 | 3A4 |
| ATOM | 567 | OE1 | GLU | 121 | 29.800 | 8.241  | 32.594 | 1.00 | 0.00 | 3A4 |
| ATOM | 568 | OE2 | GLU | 121 | 30.631 | 8.385  | 34.649 | 1.00 | 0.00 | 3A4 |
| ATOM | 569 | C   | GLU | 121 | 33.282 | 12.104 | 32.738 | 1.00 | 0.00 | 3A4 |
| ATOM | 570 | O   | GLU | 121 | 34.307 | 11.460 | 32.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 571 | N   | ASP | 122 | 33.267 | 13.450 | 32.868 | 1.00 | 0.00 | 3A4 |
| ATOM | 572 | CA  | ASP | 122 | 34.366 | 14.255 | 33.384 | 1.00 | 0.00 | 3A4 |
| ATOM | 573 | CB  | ASP | 122 | 33.940 | 15.762 | 33.320 | 1.00 | 0.00 | 3A4 |
| ATOM | 574 | CG  | ASP | 122 | 35.057 | 16.786 | 33.606 | 1.00 | 0.00 | 3A4 |
| ATOM | 575 | OD1 | ASP | 122 | 34.911 | 17.556 | 34.593 | 1.00 | 0.00 | 3A4 |
| ATOM | 576 | OD2 | ASP | 122 | 36.057 | 16.817 | 32.842 | 1.00 | 0.00 | 3A4 |
| ATOM | 577 | C   | ASP | 122 | 34.615 | 13.879 | 34.870 | 1.00 | 0.00 | 3A4 |
| ATOM | 578 | O   | ASP | 122 | 33.636 | 13.610 | 35.566 | 1.00 | 0.00 | 3A4 |
| ATOM | 579 | N   | GLU | 123 | 35.863 | 13.792 | 35.421 | 1.00 | 0.00 | 3A4 |
| ATOM | 580 | CA  | GLU | 123 | 37.162 | 14.248 | 34.972 | 1.00 | 0.00 | 3A4 |
| ATOM | 581 | CB  | GLU | 123 | 37.993 | 14.687 | 36.197 | 1.00 | 0.00 | 3A4 |
| ATOM | 582 | CG  | GLU | 123 | 37.348 | 15.854 | 36.968 | 1.00 | 0.00 | 3A4 |
| ATOM | 583 | CD  | GLU | 123 | 38.253 | 16.265 | 38.134 | 1.00 | 0.00 | 3A4 |
| ATOM | 584 | OE1 | GLU | 123 | 38.764 | 17.417 | 38.116 | 1.00 | 0.00 | 3A4 |
| ATOM | 585 | OE2 | GLU | 123 | 38.443 | 15.431 | 39.060 | 1.00 | 0.00 | 3A4 |
| ATOM | 586 | C   | GLU | 123 | 37.950 | 13.205 | 34.211 | 1.00 | 0.00 | 3A4 |
| ATOM | 587 | O   | GLU | 123 | 39.000 | 13.494 | 33.638 | 1.00 | 0.00 | 3A4 |
| ATOM | 588 | N   | GLU | 124 | 37.449 | 11.951 | 34.149 | 1.00 | 0.00 | 3A4 |
| ATOM | 589 | CA  | GLU | 124 | 38.063 | 10.827 | 33.460 | 1.00 | 0.00 | 3A4 |
| ATOM | 590 | CB  | GLU | 124 | 37.284 | 9.523  | 33.756 | 1.00 | 0.00 | 3A4 |
| ATOM | 591 | CG  | GLU | 124 | 37.186 | 9.213  | 35.261 | 1.00 | 0.00 | 3A4 |
| ATOM | 592 | CD  | GLU | 124 | 36.410 | 7.908  | 35.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 593 | OE1 | GLU | 124 | 37.010 | 6.933  | 35.993 | 1.00 | 0.00 | 3A4 |
| ATOM | 594 | OE2 | GLU | 124 | 35.204 | 7.870  | 35.096 | 1.00 | 0.00 | 3A4 |
| ATOM | 595 | C   | GLU | 124 | 38.109 | 11.000 | 31.965 | 1.00 | 0.00 | 3A4 |
| ATOM | 596 | O   | GLU | 124 | 39.087 | 10.727 | 31.279 | 1.00 | 0.00 | 3A4 |
| ATOM | 597 | N   | TRP | 125 | 37.027 | 11.579 | 31.425 | 1.00 | 0.00 | 3A4 |
| ATOM | 598 | CA  | TRP | 125 | 36.896 | 11.901 | 30.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 599 | CB  | TRP | 125 | 35.456 | 12.317 | 29.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 600 | CG  | TRP | 125 | 35.096 | 13.136 | 28.553 | 1.00 | 0.00 | 3A4 |
| ATOM | 601 | CD2 | TRP | 125 | 34.736 | 14.501 | 28.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 602 | CD1 | TRP | 125 | 34.423 | 12.765 | 27.428 | 1.00 | 0.00 | 3A4 |
| ATOM | 603 | NE1 | TRP | 125 | 33.701 | 13.815 | 26.942 | 1.00 | 0.00 | 3A4 |
| ATOM | 604 | CE2 | TRP | 125 | 33.805 | 14.860 | 27.829 | 1.00 | 0.00 | 3A4 |
| ATOM | 605 | CE3 | TRP | 125 | 35.040 | 15.361 | 29.870 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |        |      |      |     |
|------|-----|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 606 | CZ2 | TRP | 125 | 33.124 | 16.059 | 27.921 | 1.00 | 0.00 | 3A4 |
| ATOM | 607 | CZ3 | TRP | 125 | 34.396 | 16.599 | 29.921 | 1.00 | 0.00 | 3A4 |
| ATOM | 608 | CH2 | TRP | 125 | 33.421 | 16.924 | 28.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 609 | C   | TRP | 125 | 37.893 | 12.940 | 29.585 | 1.00 | 0.00 | 3A4 |
| ATOM | 610 | O   | TRP | 125 | 38.564 | 12.734 | 28.590 | 1.00 | 0.00 | 3A4 |
| ATOM | 611 | N   | LYS | 126 | 38.066 | 14.068 | 30.315 | 1.00 | 0.00 | 3A4 |
| ATOM | 612 | CA  | LYS | 126 | 38.948 | 15.161 | 29.915 | 1.00 | 0.00 | 3A4 |
| ATOM | 613 | CB  | LYS | 126 | 38.776 | 16.362 | 30.855 | 1.00 | 0.00 | 3A4 |
| ATOM | 614 | CG  | LYS | 126 | 39.424 | 17.682 | 30.406 | 1.00 | 0.00 | 3A4 |
| ATOM | 615 | CD  | LYS | 126 | 39.026 | 18.858 | 31.300 | 1.00 | 0.00 | 3A4 |
| ATOM | 616 | CE  | LYS | 126 | 39.634 | 20.191 | 30.845 | 1.00 | 0.00 | 3A4 |
| ATOM | 617 | NZ  | LYS | 126 | 39.206 | 21.296 | 31.735 | 1.00 | 0.00 | 3A4 |
| ATOM | 618 | C   | LYS | 126 | 40.413 | 14.775 | 29.867 | 1.00 | 0.00 | 3A4 |
| ATOM | 619 | O   | LYS | 126 | 41.152 | 15.173 | 28.977 | 1.00 | 0.00 | 3A4 |
| ATOM | 620 | N   | ARG | 127 | 40.830 | 13.884 | 30.785 | 1.00 | 0.00 | 3A4 |
| ATOM | 621 | CA  | ARG | 127 | 42.152 | 13.315 | 30.821 | 1.00 | 0.00 | 3A4 |
| ATOM | 622 | CB  | ARG | 127 | 42.369 | 12.556 | 32.148 | 1.00 | 0.00 | 3A4 |
| ATOM | 623 | CG  | ARG | 127 | 42.319 | 13.460 | 33.385 | 1.00 | 0.00 | 3A4 |
| ATOM | 624 | CD  | ARG | 127 | 42.230 | 12.652 | 34.686 | 1.00 | 0.00 | 3A4 |
| ATOM | 625 | NE  | ARG | 127 | 42.079 | 13.613 | 35.835 | 1.00 | 0.00 | 3A4 |
| ATOM | 626 | CZ  | ARG | 127 | 41.521 | 13.267 | 37.040 | 1.00 | 0.00 | 3A4 |
| ATOM | 627 | NH1 | ARG | 127 | 41.438 | 14.206 | 38.026 | 1.00 | 0.00 | 3A4 |
| ATOM | 628 | NH2 | ARG | 127 | 41.040 | 12.009 | 37.276 | 1.00 | 0.00 | 3A4 |
| ATOM | 629 | C   | ARG | 127 | 42.448 | 12.378 | 29.678 | 1.00 | 0.00 | 3A4 |
| ATOM | 630 | O   | ARG | 127 | 43.503 | 12.464 | 29.060 | 1.00 | 0.00 | 3A4 |
| ATOM | 631 | N   | LEU | 128 | 41.487 | 11.489 | 29.329 | 1.00 | 0.00 | 3A4 |
| ATOM | 632 | CA  | LEU | 128 | 41.614 | 10.553 | 28.227 | 1.00 | 0.00 | 3A4 |
| ATOM | 633 | CB  | LEU | 128 | 40.552 | 9.436  | 28.305 | 1.00 | 0.00 | 3A4 |
| ATOM | 634 | CG  | LEU | 128 | 40.710 | 8.475  | 29.510 | 1.00 | 0.00 | 3A4 |
| ATOM | 635 | CD1 | LEU | 128 | 39.492 | 7.536  | 29.620 | 1.00 | 0.00 | 3A4 |
| ATOM | 636 | CD2 | LEU | 128 | 42.026 | 7.670  | 29.503 | 1.00 | 0.00 | 3A4 |
| ATOM | 637 | C   | LEU | 128 | 41.513 | 11.260 | 26.900 | 1.00 | 0.00 | 3A4 |
| ATOM | 638 | O   | LEU | 128 | 42.307 | 10.998 | 26.016 | 1.00 | 0.00 | 3A4 |
| ATOM | 639 | N   | ARG | 129 | 40.613 | 12.256 | 26.764 | 1.00 | 0.00 | 3A4 |
| ATOM | 640 | CA  | ARG | 129 | 40.455 | 13.056 | 25.570 | 1.00 | 0.00 | 3A4 |
| ATOM | 641 | CB  | ARG | 129 | 39.248 | 13.995 | 25.706 | 1.00 | 0.00 | 3A4 |
| ATOM | 642 | CG  | ARG | 129 | 38.865 | 14.698 | 24.411 | 1.00 | 0.00 | 3A4 |
| ATOM | 643 | CD  | ARG | 129 | 37.443 | 15.285 | 24.477 | 1.00 | 0.00 | 3A4 |
| ATOM | 644 | NE  | ARG | 129 | 36.965 | 15.632 | 23.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 645 | CZ  | ARG | 129 | 37.094 | 16.870 | 22.512 | 1.00 | 0.00 | 3A4 |
| ATOM | 646 | NH1 | ARG | 129 | 36.589 | 17.069 | 21.260 | 1.00 | 0.00 | 3A4 |
| ATOM | 647 | NH2 | ARG | 129 | 37.709 | 17.907 | 23.155 | 1.00 | 0.00 | 3A4 |
| ATOM | 648 | C   | ARG | 129 | 41.673 | 13.896 | 25.247 | 1.00 | 0.00 | 3A4 |
| ATOM | 649 | O   | ARG | 129 | 42.125 | 13.963 | 24.109 | 1.00 | 0.00 | 3A4 |
| ATOM | 650 | N   | SER | 130 | 42.292 | 14.491 | 26.294 | 1.00 | 0.00 | 3A4 |
| ATOM | 651 | CA  | SER | 130 | 43.486 | 15.299 | 26.191 | 1.00 | 0.00 | 3A4 |
| ATOM | 652 | CB  | SER | 130 | 43.870 | 16.030 | 27.515 | 1.00 | 0.00 | 3A4 |
| ATOM | 653 | OG  | SER | 130 | 42.925 | 17.049 | 27.812 | 1.00 | 0.00 | 3A4 |
| ATOM | 654 | C   | SER | 130 | 44.691 | 14.547 | 25.703 | 1.00 | 0.00 | 3A4 |
| ATOM | 655 | O   | SER | 130 | 45.506 | 15.121 | 25.002 | 1.00 | 0.00 | 3A4 |
| ATOM | 656 | N   | LEU | 131 | 44.822 | 13.241 | 26.004 | 1.00 | 0.00 | 3A4 |
| ATOM | 657 | CA  | LEU | 131 | 45.894 | 12.396 | 25.508 | 1.00 | 0.00 | 3A4 |
| ATOM | 658 | CB  | LEU | 131 | 45.835 | 11.013 | 26.195 | 1.00 | 0.00 | 3A4 |
| ATOM | 659 | CG  | LEU | 131 | 46.473 | 11.008 | 27.591 | 1.00 | 0.00 | 3A4 |
| ATOM | 660 | CD1 | LEU | 131 | 45.836 | 9.924  | 28.474 | 1.00 | 0.00 | 3A4 |
| ATOM | 661 | CD2 | LEU | 131 | 48.005 | 10.845 | 27.482 | 1.00 | 0.00 | 3A4 |
| ATOM | 662 | C   | LEU | 131 | 45.875 | 12.189 | 24.006 | 1.00 | 0.00 | 3A4 |
| ATOM | 663 | O   | LEU | 131 | 46.913 | 12.177 | 23.361 | 1.00 | 0.00 | 3A4 |
| ATOM | 664 | N   | LEU | 132 | 44.675 | 12.059 | 23.421 | 1.00 | 0.00 | 3A4 |
| ATOM | 665 | CA  | LEU | 132 | 44.436 | 11.692 | 22.040 | 1.00 | 0.00 | 3A4 |
| ATOM | 666 | CB  | LEU | 132 | 43.113 | 10.883 | 21.884 | 1.00 | 0.00 | 3A4 |
| ATOM | 667 | CG  | LEU | 132 | 42.628 | 10.220 | 23.187 | 1.00 | 0.00 | 3A4 |
| ATOM | 668 | CD1 | LEU | 132 | 41.170 | 9.739  | 23.225 | 1.00 | 0.00 | 3A4 |
| ATOM | 669 | CD2 | LEU | 132 | 43.579 | 9.147  | 23.759 | 1.00 | 0.00 | 3A4 |
| ATOM | 670 | C   | LEU | 132 | 44.339 | 12.896 | 21.142 | 1.00 | 0.00 | 3A4 |
| ATOM | 671 | O   | LEU | 132 | 44.709 | 12.862 | 19.975 | 1.00 | 0.00 | 3A4 |
| ATOM | 672 | N   | SER | 133 | 43.808 | 14.009 | 21.685 | 1.00 | 0.00 | 3A4 |
| ATOM | 673 | CA  | SER | 133 | 43.570 | 15.239 | 20.967 | 1.00 | 0.00 | 3A4 |
| ATOM | 674 | CB  | SER | 133 | 42.882 | 16.277 | 21.854 | 1.00 | 0.00 | 3A4 |
| ATOM | 675 | OG  | SER | 133 | 43.525 | 16.664 | 23.058 | 1.00 | 0.00 | 3A4 |
| ATOM | 676 | C   | SER | 133 | 44.766 | 15.878 | 20.280 | 1.00 | 0.00 | 3A4 |
| ATOM | 677 | O   | SER | 133 | 44.586 | 16.429 | 19.192 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |        |      |      |     |
|------|-----|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 678 | N   | PRO | 134 | 46.017 | 15.798 | 20.777 | 1.00 | 0.00 | 3A4 |
| ATOM | 679 | CA  | PRO | 134 | 47.159 | 16.327 | 20.076 | 1.00 | 0.00 | 3A4 |
| ATOM | 680 | CD  | PRO | 134 | 46.405 | 15.537 | 22.155 | 1.00 | 0.00 | 3A4 |
| ATOM | 681 | CB  | PRO | 134 | 48.327 | 16.318 | 21.087 | 1.00 | 0.00 | 3A4 |
| ATOM | 682 | CG  | PRO | 134 | 47.635 | 16.387 | 22.434 | 1.00 | 0.00 | 3A4 |
| ATOM | 683 | C   | PRO | 134 | 47.567 | 15.563 | 18.844 | 1.00 | 0.00 | 3A4 |
| ATOM | 684 | O   | PRO | 134 | 48.106 | 16.175 | 17.927 | 1.00 | 0.00 | 3A4 |
| ATOM | 685 | N   | THR | 135 | 47.305 | 14.235 | 18.803 | 1.00 | 0.00 | 3A4 |
| ATOM | 686 | CA  | THR | 135 | 47.657 | 13.342 | 17.727 | 1.00 | 0.00 | 3A4 |
| ATOM | 687 | CB  | THR | 135 | 47.864 | 11.912 | 18.232 | 1.00 | 0.00 | 3A4 |
| ATOM | 688 | OG1 | THR | 135 | 46.681 | 11.299 | 18.729 | 1.00 | 0.00 | 3A4 |
| ATOM | 689 | CG2 | THR | 135 | 48.889 | 11.953 | 19.387 | 1.00 | 0.00 | 3A4 |
| ATOM | 690 | C   | THR | 135 | 46.639 | 13.419 | 16.594 | 1.00 | 0.00 | 3A4 |
| ATOM | 691 | O   | THR | 135 | 46.921 | 13.057 | 15.460 | 1.00 | 0.00 | 3A4 |
| ATOM | 692 | N   | PHE | 136 | 45.420 | 13.916 | 16.895 | 1.00 | 0.00 | 3A4 |
| ATOM | 693 | CA  | PHE | 136 | 44.322 | 13.979 | 15.962 | 1.00 | 0.00 | 3A4 |
| ATOM | 694 | CB  | PHE | 136 | 43.007 | 13.434 | 16.581 | 1.00 | 0.00 | 3A4 |
| ATOM | 695 | CG  | PHE | 136 | 43.069 | 12.028 | 17.109 | 1.00 | 0.00 | 3A4 |
| ATOM | 696 | CD1 | PHE | 136 | 42.397 | 11.733 | 18.297 | 1.00 | 0.00 | 3A4 |
| ATOM | 697 | CD2 | PHE | 136 | 43.793 | 10.992 | 16.495 | 1.00 | 0.00 | 3A4 |
| ATOM | 698 | CE1 | PHE | 136 | 42.237 | 10.417 | 18.717 | 1.00 | 0.00 | 3A4 |
| ATOM | 699 | CE2 | PHE | 136 | 43.668 | 9.665  | 16.926 | 1.00 | 0.00 | 3A4 |
| ATOM | 700 | CZ  | PHE | 136 | 42.847 | 9.372  | 18.017 | 1.00 | 0.00 | 3A4 |
| ATOM | 701 | C   | PHE | 136 | 44.074 | 15.402 | 15.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 702 | O   | PHE | 136 | 42.971 | 15.703 | 15.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 703 | N   | THR | 137 | 45.088 | 16.323 | 15.493 | 1.00 | 0.00 | 3A4 |
| ATOM | 704 | CA  | THR | 137 | 44.944 | 17.764 | 15.224 | 1.00 | 0.00 | 3A4 |
| ATOM | 705 | CB  | THR | 137 | 46.098 | 18.572 | 15.830 | 1.00 | 0.00 | 3A4 |
| ATOM | 706 | OG1 | THR | 137 | 46.156 | 18.321 | 17.228 | 1.00 | 0.00 | 3A4 |
| ATOM | 707 | CG2 | THR | 137 | 45.936 | 20.108 | 15.640 | 1.00 | 0.00 | 3A4 |
| ATOM | 708 | C   | THR | 137 | 44.796 | 18.094 | 13.739 | 1.00 | 0.00 | 3A4 |
| ATOM | 709 | O   | THR | 137 | 43.885 | 18.830 | 13.359 | 1.00 | 0.00 | 3A4 |
| ATOM | 710 | N   | SER | 138 | 45.685 | 17.534 | 12.870 | 1.00 | 0.00 | 3A4 |
| ATOM | 711 | CA  | SER | 138 | 45.656 | 17.677 | 11.419 | 1.00 | 0.00 | 3A4 |
| ATOM | 712 | CB  | SER | 138 | 47.076 | 17.874 | 10.806 | 1.00 | 0.00 | 3A4 |
| ATOM | 713 | OG  | SER | 138 | 47.648 | 19.086 | 11.280 | 1.00 | 0.00 | 3A4 |
| ATOM | 714 | C   | SER | 138 | 45.012 | 16.431 | 10.860 | 1.00 | 0.00 | 3A4 |
| ATOM | 715 | O   | SER | 138 | 43.868 | 16.450 | 10.408 | 1.00 | 0.00 | 3A4 |
| ATOM | 716 | N   | GLY | 139 | 45.756 | 15.304 | 10.953 | 1.00 | 0.00 | 3A4 |
| ATOM | 717 | CA  | GLY | 139 | 45.288 | 13.957 | 10.734 | 1.00 | 0.00 | 3A4 |
| ATOM | 718 | C   | GLY | 139 | 45.698 | 13.207 | 11.960 | 1.00 | 0.00 | 3A4 |
| ATOM | 719 | O   | GLY | 139 | 46.061 | 13.818 | 12.961 | 1.00 | 0.00 | 3A4 |
| ATOM | 720 | N   | LYS | 140 | 45.629 | 11.847 | 11.918 | 1.00 | 0.00 | 3A4 |
| ATOM | 721 | CA  | LYS | 140 | 45.777 | 10.945 | 13.054 | 1.00 | 0.00 | 3A4 |
| ATOM | 722 | CB  | LYS | 140 | 44.729 | 9.786  | 13.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 723 | CG  | LYS | 140 | 43.246 | 10.097 | 13.336 | 1.00 | 0.00 | 3A4 |
| ATOM | 724 | CD  | LYS | 140 | 42.846 | 11.560 | 13.252 | 1.00 | 0.00 | 3A4 |
| ATOM | 725 | CE  | LYS | 140 | 41.456 | 11.872 | 13.770 | 1.00 | 0.00 | 3A4 |
| ATOM | 726 | NZ  | LYS | 140 | 41.193 | 13.331 | 13.606 | 1.00 | 0.00 | 3A4 |
| ATOM | 727 | C   | LYS | 140 | 47.165 | 10.340 | 13.065 | 1.00 | 0.00 | 3A4 |
| ATOM | 728 | O   | LYS | 140 | 47.330 | 9.123  | 12.976 | 1.00 | 0.00 | 3A4 |
| ATOM | 729 | N   | LEU | 141 | 48.195 | 11.212 | 13.185 | 1.00 | 0.00 | 3A4 |
| ATOM | 730 | CA  | LEU | 141 | 49.585 | 10.835 | 13.207 | 1.00 | 0.00 | 3A4 |
| ATOM | 731 | CB  | LEU | 141 | 50.096 | 10.321 | 11.825 | 1.00 | 0.00 | 3A4 |
| ATOM | 732 | CG  | LEU | 141 | 51.411 | 9.530  | 11.812 | 1.00 | 0.00 | 3A4 |
| ATOM | 733 | CD1 | LEU | 141 | 52.059 | 9.603  | 10.425 | 1.00 | 0.00 | 3A4 |
| ATOM | 734 | CD2 | LEU | 141 | 51.161 | 8.066  | 12.211 | 1.00 | 0.00 | 3A4 |
| ATOM | 735 | C   | LEU | 141 | 50.286 | 12.100 | 13.623 | 1.00 | 0.00 | 3A4 |
| ATOM | 736 | O   | LEU | 141 | 50.455 | 12.362 | 14.813 | 1.00 | 0.00 | 3A4 |
| ATOM | 737 | N   | LYS | 142 | 50.687 | 12.924 | 12.618 | 1.00 | 0.00 | 3A4 |
| ATOM | 738 | CA  | LYS | 142 | 51.307 | 14.222 | 12.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 739 | CB  | LYS | 142 | 52.868 | 14.192 | 12.729 | 1.00 | 0.00 | 3A4 |
| ATOM | 740 | CG  | LYS | 142 | 53.516 | 13.465 | 13.915 | 1.00 | 0.00 | 3A4 |
| ATOM | 741 | CD  | LYS | 142 | 55.045 | 13.555 | 13.916 | 1.00 | 0.00 | 3A4 |
| ATOM | 742 | CE  | LYS | 142 | 55.714 | 12.858 | 15.108 | 1.00 | 0.00 | 3A4 |
| ATOM | 743 | NZ  | LYS | 142 | 55.454 | 11.401 | 15.086 | 1.00 | 0.00 | 3A4 |
| ATOM | 744 | C   | LYS | 142 | 50.813 | 15.068 | 11.606 | 1.00 | 0.00 | 3A4 |
| ATOM | 745 | O   | LYS | 142 | 50.704 | 16.287 | 11.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 746 | N   | GLU | 143 | 50.529 | 14.432 | 10.433 | 1.00 | 0.00 | 3A4 |
| ATOM | 747 | CA  | GLU | 143 | 50.169 | 15.105 | 9.198  | 1.00 | 0.00 | 3A4 |
| ATOM | 748 | CB  | GLU | 143 | 51.389 | 15.242 | 8.234  | 1.00 | 0.00 | 3A4 |
| ATOM | 749 | CG  | GLU | 143 | 51.158 | 16.046 | 6.935  | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |        |      |      |     |
|------|-----|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 750 | CD  | GLU | 143 | 50.774 | 17.493 | 7.267  | 1.00 | 0.00 | 3A4 |
| ATOM | 751 | OE1 | GLU | 143 | 51.602 | 18.194 | 7.909  | 1.00 | 0.00 | 3A4 |
| ATOM | 752 | OE2 | GLU | 143 | 49.651 | 17.917 | 6.882  | 1.00 | 0.00 | 3A4 |
| ATOM | 753 | C   | GLU | 143 | 49.047 | 14.324 | 8.559  | 1.00 | 0.00 | 3A4 |
| ATOM | 754 | O   | GLU | 143 | 47.898 | 14.760 | 8.605  | 1.00 | 0.00 | 3A4 |
| ATOM | 755 | N   | MET | 144 | 49.393 | 13.160 | 7.926  | 1.00 | 0.00 | 3A4 |
| ATOM | 756 | CA  | MET | 144 | 48.584 | 12.130 | 7.300  | 1.00 | 0.00 | 3A4 |
| ATOM | 757 | CB  | MET | 144 | 47.303 | 11.759 | 8.070  | 1.00 | 0.00 | 3A4 |
| ATOM | 758 | CG  | MET | 144 | 47.567 | 10.932 | 9.334  | 1.00 | 0.00 | 3A4 |
| ATOM | 759 | SD  | MET | 144 | 48.269 | 9.267  | 9.019  | 1.00 | 0.00 | 3A4 |
| ATOM | 760 | CE  | MET | 144 | 47.029 | 8.504  | 7.928  | 1.00 | 0.00 | 3A4 |
| ATOM | 761 | C   | MET | 144 | 48.192 | 12.409 | 5.879  | 1.00 | 0.00 | 3A4 |
| ATOM | 762 | O   | MET | 144 | 47.891 | 11.472 | 5.150  | 1.00 | 0.00 | 3A4 |
| ATOM | 763 | N   | VAL | 145 | 48.169 | 13.678 | 5.428  | 1.00 | 0.00 | 3A4 |
| ATOM | 764 | CA  | VAL | 145 | 47.650 | 14.088 | 4.130  | 1.00 | 0.00 | 3A4 |
| ATOM | 765 | CB  | VAL | 145 | 47.693 | 15.597 | 3.949  | 1.00 | 0.00 | 3A4 |
| ATOM | 766 | CG1 | VAL | 145 | 46.839 | 16.061 | 2.734  | 1.00 | 0.00 | 3A4 |
| ATOM | 767 | CG2 | VAL | 145 | 47.128 | 16.245 | 5.237  | 1.00 | 0.00 | 3A4 |
| ATOM | 768 | C   | VAL | 145 | 48.261 | 13.425 | 2.906  | 1.00 | 0.00 | 3A4 |
| ATOM | 769 | O   | VAL | 145 | 47.501 | 13.014 | 2.026  | 1.00 | 0.00 | 3A4 |
| ATOM | 770 | N   | PRO | 146 | 49.595 | 13.235 | 2.821  | 1.00 | 0.00 | 3A4 |
| ATOM | 771 | CA  | PRO | 146 | 50.226 | 12.490 | 1.741  | 1.00 | 0.00 | 3A4 |
| ATOM | 772 | CD  | PRO | 146 | 50.623 | 13.942 | 3.599  | 1.00 | 0.00 | 3A4 |
| ATOM | 773 | CB  | PRO | 146 | 51.743 | 12.625 | 1.988  | 1.00 | 0.00 | 3A4 |
| ATOM | 774 | CG  | PRO | 146 | 51.872 | 13.954 | 2.721  | 1.00 | 0.00 | 3A4 |
| ATOM | 775 | C   | PRO | 146 | 49.826 | 11.029 | 1.698  | 1.00 | 0.00 | 3A4 |
| ATOM | 776 | O   | PRO | 146 | 49.678 | 10.483 | 0.613  | 1.00 | 0.00 | 3A4 |
| ATOM | 777 | N   | ILE | 147 | 49.572 | 10.388 | 2.863  | 1.00 | 0.00 | 3A4 |
| ATOM | 778 | CA  | ILE | 147 | 49.098 | 9.027  | 2.976  | 1.00 | 0.00 | 3A4 |
| ATOM | 779 | CB  | ILE | 147 | 49.254 | 8.469  | 4.382  | 1.00 | 0.00 | 3A4 |
| ATOM | 780 | CG2 | ILE | 147 | 48.993 | 6.930  | 4.422  | 1.00 | 0.00 | 3A4 |
| ATOM | 781 | CG1 | ILE | 147 | 50.685 | 8.809  | 4.901  | 1.00 | 0.00 | 3A4 |
| ATOM | 782 | CD  | ILE | 147 | 51.018 | 8.281  | 6.300  | 1.00 | 0.00 | 3A4 |
| ATOM | 783 | C   | ILE | 147 | 47.660 | 8.881  | 2.564  | 1.00 | 0.00 | 3A4 |
| ATOM | 784 | O   | ILE | 147 | 47.306 | 7.899  | 1.922  | 1.00 | 0.00 | 3A4 |
| ATOM | 785 | N   | ILE | 148 | 46.789 | 9.866  | 2.875  | 1.00 | 0.00 | 3A4 |
| ATOM | 786 | CA  | ILE | 148 | 45.386 | 9.833  | 2.503  | 1.00 | 0.00 | 3A4 |
| ATOM | 787 | CB  | ILE | 148 | 44.570 | 10.932 | 3.172  | 1.00 | 0.00 | 3A4 |
| ATOM | 788 | CG2 | ILE | 148 | 43.057 | 10.768 | 2.811  | 1.00 | 0.00 | 3A4 |
| ATOM | 789 | CG1 | ILE | 148 | 44.675 | 10.809 | 4.718  | 1.00 | 0.00 | 3A4 |
| ATOM | 790 | CD  | ILE | 148 | 44.158 | 12.030 | 5.488  | 1.00 | 0.00 | 3A4 |
| ATOM | 791 | C   | ILE | 148 | 45.218 | 9.888  | 1.005  | 1.00 | 0.00 | 3A4 |
| ATOM | 792 | O   | ILE | 148 | 44.486 | 9.106  | 0.407  | 1.00 | 0.00 | 3A4 |
| ATOM | 793 | N   | ALA | 149 | 46.000 | 10.765 | 0.350  | 1.00 | 0.00 | 3A4 |
| ATOM | 794 | CA  | ALA | 149 | 46.058 | 10.923 | -1.086 | 1.00 | 0.00 | 3A4 |
| ATOM | 795 | CB  | ALA | 149 | 46.983 | 12.097 | -1.414 | 1.00 | 0.00 | 3A4 |
| ATOM | 796 | C   | ALA | 149 | 46.539 | 9.682  | -1.803 | 1.00 | 0.00 | 3A4 |
| ATOM | 797 | O   | ALA | 149 | 45.965 | 9.246  | -2.797 | 1.00 | 0.00 | 3A4 |
| ATOM | 798 | N   | GLN | 150 | 47.578 | 9.019  | -1.243 | 1.00 | 0.00 | 3A4 |
| ATOM | 799 | CA  | GLN | 150 | 48.121 | 7.780  | -1.753 | 1.00 | 0.00 | 3A4 |
| ATOM | 800 | CB  | GLN | 150 | 49.342 | 7.295  | -0.954 | 1.00 | 0.00 | 3A4 |
| ATOM | 801 | CG  | GLN | 150 | 50.637 | 8.037  | -1.297 | 1.00 | 0.00 | 3A4 |
| ATOM | 802 | CD  | GLN | 150 | 51.737 | 7.586  | -0.326 | 1.00 | 0.00 | 3A4 |
| ATOM | 803 | OE1 | GLN | 150 | 52.080 | 6.406  | -0.292 | 1.00 | 0.00 | 3A4 |
| ATOM | 804 | NE2 | GLN | 150 | 52.300 | 8.525  | 0.483  | 1.00 | 0.00 | 3A4 |
| ATOM | 805 | C   | GLN | 150 | 47.129 | 6.663  | -1.774 | 1.00 | 0.00 | 3A4 |
| ATOM | 806 | O   | GLN | 150 | 46.962 | 5.992  | -2.789 | 1.00 | 0.00 | 3A4 |
| ATOM | 807 | N   | TYR | 151 | 46.371 | 6.500  | -0.658 | 1.00 | 0.00 | 3A4 |
| ATOM | 808 | CA  | TYR | 151 | 45.418 | 5.431  | -0.538 | 1.00 | 0.00 | 3A4 |
| ATOM | 809 | CB  | TYR | 151 | 44.853 | 5.227  | 0.859  | 1.00 | 0.00 | 3A4 |
| ATOM | 810 | CG  | TYR | 151 | 44.181 | 3.823  | 0.880  | 1.00 | 0.00 | 3A4 |
| ATOM | 811 | CD1 | TYR | 151 | 43.188 | 3.417  | 1.745  | 1.00 | 0.00 | 3A4 |
| ATOM | 812 | CD2 | TYR | 151 | 44.795 | 2.750  | 0.124  | 1.00 | 0.00 | 3A4 |
| ATOM | 813 | CE1 | TYR | 151 | 42.443 | 2.274  | 1.345  | 1.00 | 0.00 | 3A4 |
| ATOM | 814 | CE2 | TYR | 151 | 44.170 | 1.533  | -0.113 | 1.00 | 0.00 | 3A4 |
| ATOM | 815 | CZ  | TYR | 151 | 42.935 | 1.315  | 0.454  | 1.00 | 0.00 | 3A4 |
| ATOM | 816 | OH  | TYR | 151 | 42.254 | 0.104  | 0.201  | 1.00 | 0.00 | 3A4 |
| ATOM | 817 | C   | TYR | 151 | 44.221 | 5.669  | -1.449 | 1.00 | 0.00 | 3A4 |
| ATOM | 818 | O   | TYR | 151 | 43.738 | 4.750  | -2.103 | 1.00 | 0.00 | 3A4 |
| ATOM | 819 | N   | GLY | 152 | 43.775 | 6.936  | -1.554 | 1.00 | 0.00 | 3A4 |
| ATOM | 820 | CA  | GLY | 152 | 42.703 | 7.368  | -2.423 | 1.00 | 0.00 | 3A4 |
| ATOM | 821 | C   | GLY | 152 | 42.962 | 7.025  | -3.877 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |         |      |      |     |
|------|-----|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 822 | O   | GLY | 152 | 42.122 | 6.466  | -4.565  | 1.00 | 0.00 | 3A4 |
| ATOM | 823 | N   | ASP | 153 | 44.194 | 7.284  | -4.339  | 1.00 | 0.00 | 3A4 |
| ATOM | 824 | CA  | ASP | 153 | 44.647 | 6.996  | -5.674  | 1.00 | 0.00 | 3A4 |
| ATOM | 825 | CB  | ASP | 153 | 46.061 | 7.586  | -5.844  | 1.00 | 0.00 | 3A4 |
| ATOM | 826 | CG  | ASP | 153 | 45.993 | 9.119  | -5.945  | 1.00 | 0.00 | 3A4 |
| ATOM | 827 | OD1 | ASP | 153 | 45.014 | 9.650  | -6.534  | 1.00 | 0.00 | 3A4 |
| ATOM | 828 | OD2 | ASP | 153 | 46.922 | 9.784  | -5.416  | 1.00 | 0.00 | 3A4 |
| ATOM | 829 | C   | ASP | 153 | 44.703 | 5.521  | -6.007  | 1.00 | 0.00 | 3A4 |
| ATOM | 830 | O   | ASP | 153 | 44.288 | 5.096  | -7.076  | 1.00 | 0.00 | 3A4 |
| ATOM | 831 | N   | VAL | 154 | 45.154 | 4.686  | -5.048  | 1.00 | 0.00 | 3A4 |
| ATOM | 832 | CA  | VAL | 154 | 45.173 | 3.235  | -5.160  | 1.00 | 0.00 | 3A4 |
| ATOM | 833 | CB  | VAL | 154 | 45.878 | 2.605  | -3.968  | 1.00 | 0.00 | 3A4 |
| ATOM | 834 | CG1 | VAL | 154 | 45.770 | 1.054  | -3.875  | 1.00 | 0.00 | 3A4 |
| ATOM | 835 | CG2 | VAL | 154 | 47.373 | 2.989  | -4.067  | 1.00 | 0.00 | 3A4 |
| ATOM | 836 | C   | VAL | 154 | 43.793 | 2.651  | -5.283  | 1.00 | 0.00 | 3A4 |
| ATOM | 837 | O   | VAL | 154 | 43.531 | 1.783  | -6.112  | 1.00 | 0.00 | 3A4 |
| ATOM | 838 | N   | LEU | 155 | 42.842 | 3.184  | -4.494  | 1.00 | 0.00 | 3A4 |
| ATOM | 839 | CA  | LEU | 155 | 41.460 | 2.758  | -4.505  | 1.00 | 0.00 | 3A4 |
| ATOM | 840 | CB  | LEU | 155 | 40.697 | 3.480  | -3.395  | 1.00 | 0.00 | 3A4 |
| ATOM | 841 | CG  | LEU | 155 | 41.005 | 3.018  | -1.989  | 1.00 | 0.00 | 3A4 |
| ATOM | 842 | CD1 | LEU | 155 | 40.785 | 4.226  | -1.096  | 1.00 | 0.00 | 3A4 |
| ATOM | 843 | CD2 | LEU | 155 | 40.117 | 1.825  | -1.591  | 1.00 | 0.00 | 3A4 |
| ATOM | 844 | C   | LEU | 155 | 40.732 | 3.082  | -5.782  | 1.00 | 0.00 | 3A4 |
| ATOM | 845 | O   | LEU | 155 | 39.955 | 2.295  | -6.313  | 1.00 | 0.00 | 3A4 |
| ATOM | 846 | N   | VAL | 156 | 41.020 | 4.276  | -6.333  | 1.00 | 0.00 | 3A4 |
| ATOM | 847 | CA  | VAL | 156 | 40.441 | 4.744  | -7.564  | 1.00 | 0.00 | 3A4 |
| ATOM | 848 | CB  | VAL | 156 | 40.709 | 6.216  | -7.769  | 1.00 | 0.00 | 3A4 |
| ATOM | 849 | CG1 | VAL | 156 | 40.208 | 6.709  | -9.147  | 1.00 | 0.00 | 3A4 |
| ATOM | 850 | CG2 | VAL | 156 | 39.887 | 6.989  | -6.709  | 1.00 | 0.00 | 3A4 |
| ATOM | 851 | C   | VAL | 156 | 40.956 | 3.916  | -8.726  | 1.00 | 0.00 | 3A4 |
| ATOM | 852 | O   | VAL | 156 | 40.186 | 3.474  | -9.566  | 1.00 | 0.00 | 3A4 |
| ATOM | 853 | N   | ARG | 157 | 42.263 | 3.571  | -8.714  | 1.00 | 0.00 | 3A4 |
| ATOM | 854 | CA  | ARG | 157 | 42.881 | 2.692  | -9.687  | 1.00 | 0.00 | 3A4 |
| ATOM | 855 | CB  | ARG | 157 | 44.400 | 2.603  | -9.480  | 1.00 | 0.00 | 3A4 |
| ATOM | 856 | CG  | ARG | 157 | 45.201 | 1.988  | -10.646 | 1.00 | 0.00 | 3A4 |
| ATOM | 857 | CD  | ARG | 157 | 46.718 | 1.949  | -10.406 | 1.00 | 0.00 | 3A4 |
| ATOM | 858 | NE  | ARG | 157 | 47.008 | 0.982  | -9.282  | 1.00 | 0.00 | 3A4 |
| ATOM | 859 | CZ  | ARG | 157 | 47.582 | 1.328  | -8.084  | 1.00 | 0.00 | 3A4 |
| ATOM | 860 | NH1 | ARG | 157 | 47.753 | 0.362  | -7.136  | 1.00 | 0.00 | 3A4 |
| ATOM | 861 | NH2 | ARG | 157 | 47.975 | 2.607  | -7.807  | 1.00 | 0.00 | 3A4 |
| ATOM | 862 | C   | ARG | 157 | 42.316 | 1.305  | -9.694  | 1.00 | 0.00 | 3A4 |
| ATOM | 863 | O   | ARG | 157 | 42.062 | 0.746  | -10.749 | 1.00 | 0.00 | 3A4 |
| ATOM | 864 | N   | ASN | 158 | 42.004 | 0.746  | -8.509  | 1.00 | 0.00 | 3A4 |
| ATOM | 865 | CA  | ASN | 158 | 41.363 | -0.540 | -8.359  | 1.00 | 0.00 | 3A4 |
| ATOM | 866 | CB  | ASN | 158 | 41.312 | -0.962 | -6.875  | 1.00 | 0.00 | 3A4 |
| ATOM | 867 | CG  | ASN | 158 | 42.725 | -1.184 | -6.308  | 1.00 | 0.00 | 3A4 |
| ATOM | 868 | OD1 | ASN | 158 | 43.710 | -1.336 | -7.029  | 1.00 | 0.00 | 3A4 |
| ATOM | 869 | ND2 | ASN | 158 | 42.827 | -1.211 | -4.951  | 1.00 | 0.00 | 3A4 |
| ATOM | 870 | C   | ASN | 158 | 39.959 | -0.569 | -8.928  | 1.00 | 0.00 | 3A4 |
| ATOM | 871 | O   | ASN | 158 | 39.541 | -1.568 | -9.503  | 1.00 | 0.00 | 3A4 |
| ATOM | 872 | N   | LEU | 159 | 39.205 | 0.547  | -8.840  | 1.00 | 0.00 | 3A4 |
| ATOM | 873 | CA  | LEU | 159 | 37.900 | 0.698  | -9.460  | 1.00 | 0.00 | 3A4 |
| ATOM | 874 | CB  | LEU | 159 | 37.181 | 1.944  | -8.901  | 1.00 | 0.00 | 3A4 |
| ATOM | 875 | CG  | LEU | 159 | 36.392 | 1.845  | -7.590  | 1.00 | 0.00 | 3A4 |
| ATOM | 876 | CD1 | LEU | 159 | 35.846 | 3.252  | -7.275  | 1.00 | 0.00 | 3A4 |
| ATOM | 877 | CD2 | LEU | 159 | 35.226 | 0.844  | -7.672  | 1.00 | 0.00 | 3A4 |
| ATOM | 878 | C   | LEU | 159 | 37.986 | 0.850  | -10.979 | 1.00 | 0.00 | 3A4 |
| ATOM | 879 | O   | LEU | 159 | 37.180 | 0.311  | -11.731 | 1.00 | 0.00 | 3A4 |
| ATOM | 880 | N   | ARG | 160 | 39.032 | 1.542  | -11.475 | 1.00 | 0.00 | 3A4 |
| ATOM | 881 | CA  | ARG | 160 | 39.316 | 1.707  | -12.887 | 1.00 | 0.00 | 3A4 |
| ATOM | 882 | CB  | ARG | 160 | 40.462 | 2.697  | -13.097 | 1.00 | 0.00 | 3A4 |
| ATOM | 883 | CG  | ARG | 160 | 40.032 | 4.151  | -12.829 | 1.00 | 0.00 | 3A4 |
| ATOM | 884 | CD  | ARG | 160 | 41.097 | 5.224  | -13.106 | 1.00 | 0.00 | 3A4 |
| ATOM | 885 | NE  | ARG | 160 | 42.243 | 5.069  | -12.147 | 1.00 | 0.00 | 3A4 |
| ATOM | 886 | CZ  | ARG | 160 | 43.077 | 6.096  | -11.785 | 1.00 | 0.00 | 3A4 |
| ATOM | 887 | NH1 | ARG | 160 | 44.114 | 5.859  | -10.932 | 1.00 | 0.00 | 3A4 |
| ATOM | 888 | NH2 | ARG | 160 | 42.889 | 7.363  | -12.251 | 1.00 | 0.00 | 3A4 |
| ATOM | 889 | C   | ARG | 160 | 39.687 | 0.420  | -13.585 | 1.00 | 0.00 | 3A4 |
| ATOM | 890 | O   | ARG | 160 | 39.428 | 0.250  | -14.767 | 1.00 | 0.00 | 3A4 |
| ATOM | 891 | N   | ARG | 161 | 40.250 | -0.548 | -12.834 | 1.00 | 0.00 | 3A4 |
| ATOM | 892 | CA  | ARG | 161 | 40.597 | -1.870 | -13.293 | 1.00 | 0.00 | 3A4 |
| ATOM | 893 | CB  | ARG | 161 | 41.743 | -2.432 | -12.420 | 1.00 | 0.00 | 3A4 |

|      |     |     |     |     |        |        |         |      |      |     |
|------|-----|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 894 | CG  | ARG | 161 | 43.082 | -1.717 | -12.670 | 1.00 | 0.00 | 3A4 |
| ATOM | 895 | CD  | ARG | 161 | 44.093 | -1.838 | -11.519 | 1.00 | 0.00 | 3A4 |
| ATOM | 896 | NE  | ARG | 161 | 44.400 | -3.285 | -11.257 | 1.00 | 0.00 | 3A4 |
| ATOM | 897 | CZ  | ARG | 161 | 45.172 | -3.692 | -10.198 | 1.00 | 0.00 | 3A4 |
| ATOM | 898 | NH1 | ARG | 161 | 45.396 | -5.024 | -10.010 | 1.00 | 0.00 | 3A4 |
| ATOM | 899 | NH2 | ARG | 161 | 45.720 | -2.792 | -9.328  | 1.00 | 0.00 | 3A4 |
| ATOM | 900 | C   | ARG | 161 | 39.432 | -2.837 | -13.270 | 1.00 | 0.00 | 3A4 |
| ATOM | 901 | O   | ARG | 161 | 39.618 | -4.026 | -13.474 | 1.00 | 0.00 | 3A4 |
| ATOM | 902 | N   | GLU | 162 | 38.181 | -2.341 | -13.060 | 1.00 | 0.00 | 3A4 |
| ATOM | 903 | CA  | GLU | 162 | 36.943 | -3.106 | -13.121 | 1.00 | 0.00 | 3A4 |
| ATOM | 904 | CB  | GLU | 162 | 35.704 | -2.403 | -12.447 | 1.00 | 0.00 | 3A4 |
| ATOM | 905 | CG  | GLU | 162 | 35.006 | -1.245 | -13.229 | 1.00 | 0.00 | 3A4 |
| ATOM | 906 | CD  | GLU | 162 | 33.961 | -0.524 | -12.375 | 1.00 | 0.00 | 3A4 |
| ATOM | 907 | OE1 | GLU | 162 | 34.331 | -0.002 | -11.289 | 1.00 | 0.00 | 3A4 |
| ATOM | 908 | OE2 | GLU | 162 | 32.779 | -0.469 | -12.809 | 1.00 | 0.00 | 3A4 |
| ATOM | 909 | C   | GLU | 162 | 36.578 | -3.419 | -14.538 | 1.00 | 0.00 | 3A4 |
| ATOM | 910 | O   | GLU | 162 | 36.521 | -2.577 | -15.435 | 1.00 | 0.00 | 3A4 |
| ATOM | 911 | N   | ALA | 163 | 36.386 | -4.746 | -14.788 | 1.00 | 0.00 | 3A4 |
| ATOM | 912 | CA  | ALA | 163 | 36.408 | -5.391 | -16.091 | 1.00 | 0.00 | 3A4 |
| ATOM | 913 | CB  | ALA | 163 | 37.029 | -6.809 | -15.993 | 1.00 | 0.00 | 3A4 |
| ATOM | 914 | C   | ALA | 163 | 35.037 | -5.494 | -16.717 | 1.00 | 0.00 | 3A4 |
| ATOM | 915 | O   | ALA | 163 | 34.019 | -5.308 | -16.051 | 1.00 | 0.00 | 3A4 |
| ATOM | 916 | N   | GLU | 164 | 35.042 | -5.771 | -18.059 | 1.00 | 0.00 | 3A4 |
| ATOM | 917 | CA  | GLU | 164 | 33.935 | -5.860 | -19.009 | 1.00 | 0.00 | 3A4 |
| ATOM | 918 | CB  | GLU | 164 | 32.661 | -6.587 | -18.459 | 1.00 | 0.00 | 3A4 |
| ATOM | 919 | CG  | GLU | 164 | 31.701 | -7.151 | -19.531 | 1.00 | 0.00 | 3A4 |
| ATOM | 920 | CD  | GLU | 164 | 30.505 | -7.813 | -18.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 921 | OE1 | GLU | 164 | 29.737 | -7.082 | -18.156 | 1.00 | 0.00 | 3A4 |
| ATOM | 922 | OE2 | GLU | 164 | 30.342 | -9.055 | -18.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 923 | C   | GLU | 164 | 33.612 | -4.461 | -19.520 | 1.00 | 0.00 | 3A4 |
| ATOM | 924 | O   | GLU | 164 | 32.462 | -4.138 | -19.797 | 1.00 | 0.00 | 3A4 |
| ATOM | 925 | N   | THR | 165 | 34.671 | -3.592 | -19.572 | 1.00 | 0.00 | 3A4 |
| ATOM | 926 | CA  | THR | 165 | 34.730 | -2.131 | -19.714 | 1.00 | 0.00 | 3A4 |
| ATOM | 927 | CB  | THR | 165 | 34.039 | -1.480 | -20.938 | 1.00 | 0.00 | 3A4 |
| ATOM | 928 | OG1 | THR | 165 | 32.615 | -1.557 | -20.965 | 1.00 | 0.00 | 3A4 |
| ATOM | 929 | CG2 | THR | 165 | 34.604 | -2.115 | -22.228 | 1.00 | 0.00 | 3A4 |
| ATOM | 930 | C   | THR | 165 | 34.372 | -1.470 | -18.379 | 1.00 | 0.00 | 3A4 |
| ATOM | 931 | O   | THR | 165 | 35.235 | -0.931 | -17.690 | 1.00 | 0.00 | 3A4 |
| ATOM | 932 | N   | GLY | 166 | 33.075 | -1.547 | -17.996 | 1.00 | 0.00 | 3A4 |
| ATOM | 933 | CA  | GLY | 166 | 32.567 | -1.129 | -16.720 | 1.00 | 0.00 | 3A4 |
| ATOM | 934 | C   | GLY | 166 | 31.084 | -1.094 | -16.877 | 1.00 | 0.00 | 3A4 |
| ATOM | 935 | O   | GLY | 166 | 30.541 | -0.151 | -17.449 | 1.00 | 0.00 | 3A4 |
| ATOM | 936 | N   | LYS | 167 | 30.386 | -2.143 | -16.363 | 1.00 | 0.00 | 3A4 |
| ATOM | 937 | CA  | LYS | 167 | 28.935 | -2.211 | -16.262 | 1.00 | 0.00 | 3A4 |
| ATOM | 938 | CB  | LYS | 167 | 28.217 | -3.202 | -17.239 | 1.00 | 0.00 | 3A4 |
| ATOM | 939 | CG  | LYS | 167 | 28.165 | -2.770 | -18.713 | 1.00 | 0.00 | 3A4 |
| ATOM | 940 | CD  | LYS | 167 | 29.336 | -3.252 | -19.574 | 1.00 | 0.00 | 3A4 |
| ATOM | 941 | CE  | LYS | 167 | 29.134 | -2.949 | -21.066 | 1.00 | 0.00 | 3A4 |
| ATOM | 942 | NZ  | LYS | 167 | 30.208 | -3.554 | -21.890 | 1.00 | 0.00 | 3A4 |
| ATOM | 943 | C   | LYS | 167 | 28.582 | -2.486 | -14.802 | 1.00 | 0.00 | 3A4 |
| ATOM | 944 | O   | LYS | 167 | 27.816 | -1.688 | -14.271 | 1.00 | 0.00 | 3A4 |
| ATOM | 945 | N   | PRO | 168 | 29.041 | -3.521 | -14.057 | 1.00 | 0.00 | 3A4 |
| ATOM | 946 | CA  | PRO | 168 | 28.796 | -3.641 | -12.622 | 1.00 | 0.00 | 3A4 |
| ATOM | 947 | CD  | PRO | 168 | 29.518 | -4.787 | -14.626 | 1.00 | 0.00 | 3A4 |
| ATOM | 948 | CB  | PRO | 168 | 28.695 | -5.165 | -12.400 | 1.00 | 0.00 | 3A4 |
| ATOM | 949 | CG  | PRO | 168 | 29.625 | -5.777 | -13.459 | 1.00 | 0.00 | 3A4 |
| ATOM | 950 | C   | PRO | 168 | 29.938 | -3.027 | -11.812 | 1.00 | 0.00 | 3A4 |
| ATOM | 951 | O   | PRO | 168 | 31.100 | -3.303 | -12.110 | 1.00 | 0.00 | 3A4 |
| ATOM | 952 | N   | VAL | 169 | 29.609 | -2.275 | -10.724 | 1.00 | 0.00 | 3A4 |
| ATOM | 953 | CA  | VAL | 169 | 30.441 | -2.280 | -9.531  | 1.00 | 0.00 | 3A4 |
| ATOM | 954 | CB  | VAL | 169 | 31.674 | -1.381 | -9.591  | 1.00 | 0.00 | 3A4 |
| ATOM | 955 | CG1 | VAL | 169 | 31.356 | 0.130  | -9.641  | 1.00 | 0.00 | 3A4 |
| ATOM | 956 | CG2 | VAL | 169 | 32.702 | -1.746 | -8.502  | 1.00 | 0.00 | 3A4 |
| ATOM | 957 | C   | VAL | 169 | 29.535 | -1.926 | -8.382  | 1.00 | 0.00 | 3A4 |
| ATOM | 958 | O   | VAL | 169 | 28.623 | -1.120 | -8.526  | 1.00 | 0.00 | 3A4 |
| ATOM | 959 | N   | THR | 170 | 29.805 | -2.498 | -7.184  | 1.00 | 0.00 | 3A4 |
| ATOM | 960 | CA  | THR | 170 | 29.193 | -2.121 | -5.931  | 1.00 | 0.00 | 3A4 |
| ATOM | 961 | CB  | THR | 170 | 28.902 | -3.314 | -5.038  | 1.00 | 0.00 | 3A4 |
| ATOM | 962 | OG1 | THR | 170 | 28.066 | -4.231 | -5.734  | 1.00 | 0.00 | 3A4 |
| ATOM | 963 | CG2 | THR | 170 | 28.173 | -2.877 | -3.736  | 1.00 | 0.00 | 3A4 |
| ATOM | 964 | C   | THR | 170 | 30.178 | -1.183 | -5.305  | 1.00 | 0.00 | 3A4 |
| ATOM | 965 | O   | THR | 170 | 31.232 | -1.589 | -4.831  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 966  | N   | LEU | 171 | 29.854 | 0.126  | -5.296 | 1.00 | 0.00 | 3A4 |
| ATOM | 967  | CA  | LEU | 171 | 30.705 | 1.177  | -4.769 | 1.00 | 0.00 | 3A4 |
| ATOM | 968  | CB  | LEU | 171 | 30.055 | 2.555  | -5.044 | 1.00 | 0.00 | 3A4 |
| ATOM | 969  | CG  | LEU | 171 | 30.547 | 3.319  | -6.282 | 1.00 | 0.00 | 3A4 |
| ATOM | 970  | CD1 | LEU | 171 | 29.654 | 4.563  | -6.453 | 1.00 | 0.00 | 3A4 |
| ATOM | 971  | CD2 | LEU | 171 | 32.040 | 3.710  | -6.194 | 1.00 | 0.00 | 3A4 |
| ATOM | 972  | C   | LEU | 171 | 30.998 | 1.069  | -3.277 | 1.00 | 0.00 | 3A4 |
| ATOM | 973  | O   | LEU | 171 | 32.076 | 1.436  | -2.831 | 1.00 | 0.00 | 3A4 |
| ATOM | 974  | N   | LYS | 172 | 30.072 | 0.510  | -2.464 | 1.00 | 0.00 | 3A4 |
| ATOM | 975  | CA  | LYS | 172 | 30.261 | 0.291  | -1.041 | 1.00 | 0.00 | 3A4 |
| ATOM | 976  | CB  | LYS | 172 | 28.920 | -0.132 | -0.376 | 1.00 | 0.00 | 3A4 |
| ATOM | 977  | CG  | LYS | 172 | 28.909 | -0.334 | 1.158  | 1.00 | 0.00 | 3A4 |
| ATOM | 978  | CD  | LYS | 172 | 29.194 | 0.939  | 1.969  | 1.00 | 0.00 | 3A4 |
| ATOM | 979  | CE  | LYS | 172 | 29.078 | 0.766  | 3.488  | 1.00 | 0.00 | 3A4 |
| ATOM | 980  | NZ  | LYS | 172 | 30.110 | -0.160 | 4.012  | 1.00 | 0.00 | 3A4 |
| ATOM | 981  | C   | LYS | 172 | 31.330 | -0.744 | -0.748 | 1.00 | 0.00 | 3A4 |
| ATOM | 982  | O   | LYS | 172 | 32.274 | -0.492 | -0.010 | 1.00 | 0.00 | 3A4 |
| ATOM | 983  | N   | ASP | 173 | 31.243 | -1.937 | -1.374 | 1.00 | 0.00 | 3A4 |
| ATOM | 984  | CA  | ASP | 173 | 32.134 | -3.048 | -1.103 | 1.00 | 0.00 | 3A4 |
| ATOM | 985  | CB  | ASP | 173 | 31.447 | -4.365 | -1.539 | 1.00 | 0.00 | 3A4 |
| ATOM | 986  | CG  | ASP | 173 | 32.095 | -5.634 | -0.940 | 1.00 | 0.00 | 3A4 |
| ATOM | 987  | OD1 | ASP | 173 | 32.129 | -5.750 | 0.315  | 1.00 | 0.00 | 3A4 |
| ATOM | 988  | OD2 | ASP | 173 | 32.559 | -6.496 | -1.735 | 1.00 | 0.00 | 3A4 |
| ATOM | 989  | C   | ASP | 173 | 33.491 | -2.909 | -1.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 990  | O   | ASP | 173 | 34.487 | -3.361 | -1.199 | 1.00 | 0.00 | 3A4 |
| ATOM | 991  | N   | VAL | 174 | 33.571 | -2.272 | -2.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 992  | CA  | VAL | 174 | 34.804 | -2.128 | -3.702 | 1.00 | 0.00 | 3A4 |
| ATOM | 993  | CB  | VAL | 174 | 34.550 | -2.192 | -5.209 | 1.00 | 0.00 | 3A4 |
| ATOM | 994  | CG1 | VAL | 174 | 35.866 | -2.225 | -6.033 | 1.00 | 0.00 | 3A4 |
| ATOM | 995  | CG2 | VAL | 174 | 33.783 | -3.513 | -5.482 | 1.00 | 0.00 | 3A4 |
| ATOM | 996  | C   | VAL | 174 | 35.560 | -0.866 | -3.321 | 1.00 | 0.00 | 3A4 |
| ATOM | 997  | O   | VAL | 174 | 36.767 | -0.793 | -3.522 | 1.00 | 0.00 | 3A4 |
| ATOM | 998  | N   | PHE | 175 | 34.889 | 0.162  | -2.748 | 1.00 | 0.00 | 3A4 |
| ATOM | 999  | CA  | PHE | 175 | 35.513 | 1.457  | -2.585 | 1.00 | 0.00 | 3A4 |
| ATOM | 1000 | CB  | PHE | 175 | 34.996 | 2.458  | -3.637 | 1.00 | 0.00 | 3A4 |
| ATOM | 1001 | CG  | PHE | 175 | 35.738 | 3.789  | -3.669 | 1.00 | 0.00 | 3A4 |
| ATOM | 1002 | CD1 | PHE | 175 | 35.169 | 4.936  | -3.079 | 1.00 | 0.00 | 3A4 |
| ATOM | 1003 | CD2 | PHE | 175 | 37.019 | 3.896  | -4.239 | 1.00 | 0.00 | 3A4 |
| ATOM | 1004 | CE1 | PHE | 175 | 35.866 | 6.153  | -3.047 | 1.00 | 0.00 | 3A4 |
| ATOM | 1005 | CE2 | PHE | 175 | 37.703 | 5.120  | -4.237 | 1.00 | 0.00 | 3A4 |
| ATOM | 1006 | CZ  | PHE | 175 | 37.136 | 6.244  | -3.628 | 1.00 | 0.00 | 3A4 |
| ATOM | 1007 | C   | PHE | 175 | 35.362 | 1.997  | -1.219 | 1.00 | 0.00 | 3A4 |
| ATOM | 1008 | O   | PHE | 175 | 36.347 | 2.184  | -0.509 | 1.00 | 0.00 | 3A4 |
| ATOM | 1009 | N   | GLY | 176 | 34.105 | 2.318  | -0.836 | 1.00 | 0.00 | 3A4 |
| ATOM | 1010 | CA  | GLY | 176 | 33.755 | 3.060  | 0.352  | 1.00 | 0.00 | 3A4 |
| ATOM | 1011 | C   | GLY | 176 | 34.098 | 2.332  | 1.609  | 1.00 | 0.00 | 3A4 |
| ATOM | 1012 | O   | GLY | 176 | 34.413 | 2.958  | 2.614  | 1.00 | 0.00 | 3A4 |
| ATOM | 1013 | N   | ALA | 177 | 34.126 | 0.976  | 1.565  | 1.00 | 0.00 | 3A4 |
| ATOM | 1014 | CA  | ALA | 177 | 34.485 | 0.144  | 2.688  | 1.00 | 0.00 | 3A4 |
| ATOM | 1015 | CB  | ALA | 177 | 33.968 | -1.294 | 2.532  | 1.00 | 0.00 | 3A4 |
| ATOM | 1016 | C   | ALA | 177 | 35.962 | 0.124  | 2.957  | 1.00 | 0.00 | 3A4 |
| ATOM | 1017 | O   | ALA | 177 | 36.406 | 0.327  | 4.080  | 1.00 | 0.00 | 3A4 |
| ATOM | 1018 | N   | TYR | 178 | 36.777 | -0.058 | 1.903  | 1.00 | 0.00 | 3A4 |
| ATOM | 1019 | CA  | TYR | 178 | 38.203 | -0.242 | 2.016  | 1.00 | 0.00 | 3A4 |
| ATOM | 1020 | CB  | TYR | 178 | 38.721 | -0.724 | 0.638  | 1.00 | 0.00 | 3A4 |
| ATOM | 1021 | CG  | TYR | 178 | 38.656 | -2.235 | 0.593  | 1.00 | 0.00 | 3A4 |
| ATOM | 1022 | CD1 | TYR | 178 | 37.893 | -2.854 | -0.416 | 1.00 | 0.00 | 3A4 |
| ATOM | 1023 | CD2 | TYR | 178 | 39.236 | -3.052 | 1.584  | 1.00 | 0.00 | 3A4 |
| ATOM | 1024 | CE1 | TYR | 178 | 37.711 | -4.243 | -0.441 | 1.00 | 0.00 | 3A4 |
| ATOM | 1025 | CE2 | TYR | 178 | 39.039 | -4.442 | 1.580  | 1.00 | 0.00 | 3A4 |
| ATOM | 1026 | CZ  | TYR | 178 | 38.282 | -5.040 | 0.562  | 1.00 | 0.00 | 3A4 |
| ATOM | 1027 | OH  | TYR | 178 | 38.091 | -6.439 | 0.553  | 1.00 | 0.00 | 3A4 |
| ATOM | 1028 | C   | TYR | 178 | 38.966 | 1.017  | 2.362  | 1.00 | 0.00 | 3A4 |
| ATOM | 1029 | O   | TYR | 178 | 39.918 | 0.985  | 3.127  | 1.00 | 0.00 | 3A4 |
| ATOM | 1030 | N   | SER | 179 | 38.545 | 2.180  | 1.822  | 1.00 | 0.00 | 3A4 |
| ATOM | 1031 | CA  | SER | 179 | 39.171 | 3.471  | 2.018  | 1.00 | 0.00 | 3A4 |
| ATOM | 1032 | CB  | SER | 179 | 38.412 | 4.545  | 1.196  | 1.00 | 0.00 | 3A4 |
| ATOM | 1033 | OG  | SER | 179 | 39.108 | 5.787  | 1.074  | 1.00 | 0.00 | 3A4 |
| ATOM | 1034 | C   | SER | 179 | 39.344 | 3.878  | 3.465  | 1.00 | 0.00 | 3A4 |
| ATOM | 1035 | O   | SER | 179 | 40.445 | 4.039  | 3.966  | 1.00 | 0.00 | 3A4 |
| ATOM | 1036 | N   | MET | 180 | 38.263 | 3.919  | 4.233  | 1.00 | 0.00 | 3A4 |
| ATOM | 1037 | CA  | MET | 180 | 38.328 | 4.314  | 5.621  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 1038 | CB  | MET | 180 | 36.898 | 4.623  | 5.984  | 1.00 | 0.00 | 3A4 |
| ATOM | 1039 | CG  | MET | 180 | 36.729 | 5.941  | 5.189  | 1.00 | 0.00 | 3A4 |
| ATOM | 1040 | SD  | MET | 180 | 35.589 | 5.903  | 3.791  | 1.00 | 0.00 | 3A4 |
| ATOM | 1041 | CE  | MET | 180 | 36.564 | 7.153  | 2.893  | 1.00 | 0.00 | 3A4 |
| ATOM | 1042 | C   | MET | 180 | 38.961 | 3.325  | 6.527  | 1.00 | 0.00 | 3A4 |
| ATOM | 1043 | O   | MET | 180 | 39.602 | 3.684  | 7.513  | 1.00 | 0.00 | 3A4 |
| ATOM | 1044 | N   | ASP | 181 | 38.892 | 2.030  | 6.144  | 1.00 | 0.00 | 3A4 |
| ATOM | 1045 | CA  | ASP | 181 | 39.455 | 1.016  | 6.971  | 1.00 | 0.00 | 3A4 |
| ATOM | 1046 | CB  | ASP | 181 | 38.927 | -0.386 | 6.705  | 1.00 | 0.00 | 3A4 |
| ATOM | 1047 | CG  | ASP | 181 | 38.781 | -1.148 | 5.400  | 1.00 | 0.00 | 3A4 |
| ATOM | 1048 | OD1 | ASP | 181 | 39.773 | -1.165 | 4.635  | 1.00 | 0.00 | 3A4 |
| ATOM | 1049 | OD2 | ASP | 181 | 37.728 | -1.810 | 5.195  | 1.00 | 0.00 | 3A4 |
| ATOM | 1050 | C   | ASP | 181 | 40.963 | 0.976  | 6.884  | 1.00 | 0.00 | 3A4 |
| ATOM | 1051 | O   | ASP | 181 | 41.663 | 0.876  | 7.886  | 1.00 | 0.00 | 3A4 |
| ATOM | 1052 | N   | VAL | 182 | 41.515 | 1.163  | 5.671  | 1.00 | 0.00 | 3A4 |
| ATOM | 1053 | CA  | VAL | 182 | 42.946 | 1.238  | 5.464  | 1.00 | 0.00 | 3A4 |
| ATOM | 1054 | CB  | VAL | 182 | 43.279 | 1.227  | 4.010  | 1.00 | 0.00 | 3A4 |
| ATOM | 1055 | CG1 | VAL | 182 | 44.767 | 1.508  | 3.706  | 1.00 | 0.00 | 3A4 |
| ATOM | 1056 | CG2 | VAL | 182 | 42.889 | -0.181 | 3.532  | 1.00 | 0.00 | 3A4 |
| ATOM | 1057 | C   | VAL | 182 | 43.593 | 2.408  | 6.151  | 1.00 | 0.00 | 3A4 |
| ATOM | 1058 | O   | VAL | 182 | 44.676 | 2.298  | 6.708  | 1.00 | 0.00 | 3A4 |
| ATOM | 1059 | N   | ILE | 183 | 42.877 | 3.540  | 6.210  | 1.00 | 0.00 | 3A4 |
| ATOM | 1060 | CA  | ILE | 183 | 43.341 | 4.740  | 6.855  | 1.00 | 0.00 | 3A4 |
| ATOM | 1061 | CB  | ILE | 183 | 42.480 | 5.913  | 6.432  | 1.00 | 0.00 | 3A4 |
| ATOM | 1062 | CG2 | ILE | 183 | 42.783 | 7.205  | 7.220  | 1.00 | 0.00 | 3A4 |
| ATOM | 1063 | CG1 | ILE | 183 | 42.712 | 6.215  | 4.926  | 1.00 | 0.00 | 3A4 |
| ATOM | 1064 | CD  | ILE | 183 | 44.121 | 6.672  | 4.516  | 1.00 | 0.00 | 3A4 |
| ATOM | 1065 | C   | ILE | 183 | 43.365 | 4.589  | 8.352  | 1.00 | 0.00 | 3A4 |
| ATOM | 1066 | O   | ILE | 183 | 44.321 | 4.972  | 9.017  | 1.00 | 0.00 | 3A4 |
| ATOM | 1067 | N   | THR | 184 | 42.323 | 3.969  | 8.947  | 1.00 | 0.00 | 3A4 |
| ATOM | 1068 | CA  | THR | 184 | 42.311 | 3.780  | 10.379 | 1.00 | 0.00 | 3A4 |
| ATOM | 1069 | CB  | THR | 184 | 40.896 | 3.599  | 10.968 | 1.00 | 0.00 | 3A4 |
| ATOM | 1070 | OG1 | THR | 184 | 40.842 | 3.873  | 12.369 | 1.00 | 0.00 | 3A4 |
| ATOM | 1071 | CG2 | THR | 184 | 40.253 | 2.222  | 10.686 | 1.00 | 0.00 | 3A4 |
| ATOM | 1072 | C   | THR | 184 | 43.288 | 2.710  | 10.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 1073 | O   | THR | 184 | 43.934 | 2.838  | 11.842 | 1.00 | 0.00 | 3A4 |
| ATOM | 1074 | N   | SER | 185 | 43.544 | 1.697  | 9.955  | 1.00 | 0.00 | 3A4 |
| ATOM | 1075 | CA  | SER | 185 | 44.571 | 0.701  | 10.179 | 1.00 | 0.00 | 3A4 |
| ATOM | 1076 | CB  | SER | 185 | 44.486 | -0.452 | 9.173  | 1.00 | 0.00 | 3A4 |
| ATOM | 1077 | OG  | SER | 185 | 43.278 | -1.178 | 9.354  | 1.00 | 0.00 | 3A4 |
| ATOM | 1078 | C   | SER | 185 | 45.975 | 1.270  | 10.157 | 1.00 | 0.00 | 3A4 |
| ATOM | 1079 | O   | SER | 185 | 46.793 | 0.962  | 11.011 | 1.00 | 0.00 | 3A4 |
| ATOM | 1080 | N   | THR | 186 | 46.255 | 2.211  | 9.238  | 1.00 | 0.00 | 3A4 |
| ATOM | 1081 | CA  | THR | 186 | 47.523 | 2.905  | 9.158  | 1.00 | 0.00 | 3A4 |
| ATOM | 1082 | CB  | THR | 186 | 47.674 | 3.626  | 7.845  | 1.00 | 0.00 | 3A4 |
| ATOM | 1083 | OG1 | THR | 186 | 46.613 | 4.495  | 7.478  | 1.00 | 0.00 | 3A4 |
| ATOM | 1084 | CG2 | THR | 186 | 47.869 | 2.559  | 6.746  | 1.00 | 0.00 | 3A4 |
| ATOM | 1085 | C   | THR | 186 | 47.770 | 3.895  | 10.256 | 1.00 | 0.00 | 3A4 |
| ATOM | 1086 | O   | THR | 186 | 48.906 | 4.171  | 10.627 | 1.00 | 0.00 | 3A4 |
| ATOM | 1087 | N   | SER | 187 | 46.676 | 4.433  | 10.825 | 1.00 | 0.00 | 3A4 |
| ATOM | 1088 | CA  | SER | 187 | 46.674 | 5.311  | 11.961 | 1.00 | 0.00 | 3A4 |
| ATOM | 1089 | CB  | SER | 187 | 45.260 | 5.983  | 12.078 | 1.00 | 0.00 | 3A4 |
| ATOM | 1090 | OG  | SER | 187 | 45.037 | 6.742  | 13.262 | 1.00 | 0.00 | 3A4 |
| ATOM | 1091 | C   | SER | 187 | 47.012 | 4.556  | 13.221 | 1.00 | 0.00 | 3A4 |
| ATOM | 1092 | O   | SER | 187 | 47.753 | 5.052  | 14.047 | 1.00 | 0.00 | 3A4 |
| ATOM | 1093 | N   | PHE | 188 | 46.490 | 3.324  | 13.352 | 1.00 | 0.00 | 3A4 |
| ATOM | 1094 | CA  | PHE | 188 | 46.634 | 2.477  | 14.511 | 1.00 | 0.00 | 3A4 |
| ATOM | 1095 | CB  | PHE | 188 | 45.408 | 1.520  | 14.609 | 1.00 | 0.00 | 3A4 |
| ATOM | 1096 | CG  | PHE | 188 | 44.440 | 2.221  | 15.507 | 1.00 | 0.00 | 3A4 |
| ATOM | 1097 | CD1 | PHE | 188 | 43.828 | 3.428  | 15.112 | 1.00 | 0.00 | 3A4 |
| ATOM | 1098 | CD2 | PHE | 188 | 44.425 | 1.853  | 16.860 | 1.00 | 0.00 | 3A4 |
| ATOM | 1099 | CE1 | PHE | 188 | 43.309 | 4.298  | 16.068 | 1.00 | 0.00 | 3A4 |
| ATOM | 1100 | CE2 | PHE | 188 | 43.917 | 2.727  | 17.815 | 1.00 | 0.00 | 3A4 |
| ATOM | 1101 | CZ  | PHE | 188 | 43.370 | 3.945  | 17.418 | 1.00 | 0.00 | 3A4 |
| ATOM | 1102 | C   | PHE | 188 | 47.882 | 1.665  | 14.537 | 1.00 | 0.00 | 3A4 |
| ATOM | 1103 | O   | PHE | 188 | 48.386 | 1.332  | 15.605 | 1.00 | 0.00 | 3A4 |
| ATOM | 1104 | N   | GLY | 189 | 48.414 | 1.335  | 13.350 | 1.00 | 0.00 | 3A4 |
| ATOM | 1105 | CA  | GLY | 189 | 49.610 | 0.550  | 13.208 | 1.00 | 0.00 | 3A4 |
| ATOM | 1106 | C   | GLY | 189 | 49.281 | -0.923 | 13.101 | 1.00 | 0.00 | 3A4 |
| ATOM | 1107 | O   | GLY | 189 | 50.025 | -1.788 | 13.555 | 1.00 | 0.00 | 3A4 |
| ATOM | 1108 | N   | VAL | 190 | 48.147 | -1.240 | 12.428 | 1.00 | 0.00 | 3A4 |
| ATOM | 1109 | CA  | VAL | 190 | 47.745 | -2.576 | 12.011 | 1.00 | 0.00 | 3A4 |



|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1110 | CB  | VAL | 190 | 46.239 | -2.768  | 11.929 | 1.00 | 0.00 | 3A4 |
| ATOM | 1111 | CG1 | VAL | 190 | 45.823 | -4.253  | 11.759 | 1.00 | 0.00 | 3A4 |
| ATOM | 1112 | CG2 | VAL | 190 | 45.621 | -2.217  | 13.235 | 1.00 | 0.00 | 3A4 |
| ATOM | 1113 | C   | VAL | 190 | 48.306 | -2.843  | 10.635 | 1.00 | 0.00 | 3A4 |
| ATOM | 1114 | O   | VAL | 190 | 48.419 | -1.948  | 9.801  | 1.00 | 0.00 | 3A4 |
| ATOM | 1115 | N   | ASN | 191 | 48.675 | -4.105  | 10.372 | 1.00 | 0.00 | 3A4 |
| ATOM | 1116 | CA  | ASN | 191 | 49.636 | -4.477  | 9.377  | 1.00 | 0.00 | 3A4 |
| ATOM | 1117 | CB  | ASN | 191 | 49.869 | -5.997  | 9.517  | 1.00 | 0.00 | 3A4 |
| ATOM | 1118 | CG  | ASN | 191 | 51.211 | -6.502  | 8.934  | 1.00 | 0.00 | 3A4 |
| ATOM | 1119 | OD1 | ASN | 191 | 52.277 | -6.160  | 9.445  | 1.00 | 0.00 | 3A4 |
| ATOM | 1120 | ND2 | ASN | 191 | 51.156 | -7.322  | 7.848  | 1.00 | 0.00 | 3A4 |
| ATOM | 1121 | C   | ASN | 191 | 49.394 | -4.146  | 7.970  | 1.00 | 0.00 | 3A4 |
| ATOM | 1122 | O   | ASN | 191 | 48.268 | -4.363  | 7.523  | 1.00 | 0.00 | 3A4 |
| ATOM | 1123 | N   | ILE | 192 | 50.505 | -3.532  | 7.398  | 1.00 | 0.00 | 3A4 |
| ATOM | 1124 | CA  | ILE | 192 | 50.796 | -3.011  | 6.064  | 1.00 | 0.00 | 3A4 |
| ATOM | 1125 | CB  | ILE | 192 | 49.572 | -3.045  | 5.191  | 1.00 | 0.00 | 3A4 |
| ATOM | 1126 | CG2 | ILE | 192 | 48.539 | -2.012  | 5.843  | 1.00 | 0.00 | 3A4 |
| ATOM | 1127 | CG1 | ILE | 192 | 49.850 | -3.205  | 3.643  | 1.00 | 0.00 | 3A4 |
| ATOM | 1128 | CD  | ILE | 192 | 50.855 | -4.296  | 3.249  | 1.00 | 0.00 | 3A4 |
| ATOM | 1129 | C   | ILE | 192 | 51.332 | -1.562  | 6.101  | 1.00 | 0.00 | 3A4 |
| ATOM | 1130 | O   | ILE | 192 | 51.714 | -1.049  | 7.152  | 1.00 | 0.00 | 3A4 |
| ATOM | 1131 | N   | ASP | 193 | 51.273 | -0.876  | 4.912  | 1.00 | 0.00 | 3A4 |
| ATOM | 1132 | CA  | ASP | 193 | 51.280 | 0.551   | 4.649  | 1.00 | 0.00 | 3A4 |
| ATOM | 1133 | CB  | ASP | 193 | 52.500 | 0.950   | 3.755  | 1.00 | 0.00 | 3A4 |
| ATOM | 1134 | CG  | ASP | 193 | 52.747 | 2.473   | 3.713  | 1.00 | 0.00 | 3A4 |
| ATOM | 1135 | OD1 | ASP | 193 | 52.690 | 3.055   | 2.596  | 1.00 | 0.00 | 3A4 |
| ATOM | 1136 | OD2 | ASP | 193 | 52.993 | 3.065   | 4.798  | 1.00 | 0.00 | 3A4 |
| ATOM | 1137 | C   | ASP | 193 | 49.942 | 0.941   | 3.982  | 1.00 | 0.00 | 3A4 |
| ATOM | 1138 | O   | ASP | 193 | 49.555 | 2.107   | 4.042  | 1.00 | 0.00 | 3A4 |
| ATOM | 1139 | N   | SER | 194 | 49.199 | -0.025  | 3.351  | 1.00 | 0.00 | 3A4 |
| ATOM | 1140 | CA  | SER | 194 | 47.801 | 0.108   | 2.935  | 1.00 | 0.00 | 3A4 |
| ATOM | 1141 | CB  | SER | 194 | 47.674 | 0.859   | 1.564  | 1.00 | 0.00 | 3A4 |
| ATOM | 1142 | OG  | SER | 194 | 48.568 | 0.364   | 0.570  | 1.00 | 0.00 | 3A4 |
| ATOM | 1143 | C   | SER | 194 | 47.072 | -1.263  | 2.877  | 1.00 | 0.00 | 3A4 |
| ATOM | 1144 | O   | SER | 194 | 47.201 | -1.949  | 1.864  | 1.00 | 0.00 | 3A4 |
| ATOM | 1145 | N   | LEU | 195 | 46.300 | -1.682  | 3.968  | 1.00 | 0.00 | 3A4 |
| ATOM | 1146 | CA  | LEU | 195 | 45.506 | -2.928  | 4.205  | 1.00 | 0.00 | 3A4 |
| ATOM | 1147 | CB  | LEU | 195 | 44.616 | -3.155  | 2.908  | 1.00 | 0.00 | 3A4 |
| ATOM | 1148 | CG  | LEU | 195 | 43.358 | -4.046  | 2.893  | 1.00 | 0.00 | 3A4 |
| ATOM | 1149 | CD1 | LEU | 195 | 42.566 | -3.731  | 1.614  | 1.00 | 0.00 | 3A4 |
| ATOM | 1150 | CD2 | LEU | 195 | 43.591 | -5.569  | 2.963  | 1.00 | 0.00 | 3A4 |
| ATOM | 1151 | C   | LEU | 195 | 46.313 | -4.231  | 4.384  | 1.00 | 0.00 | 3A4 |
| ATOM | 1152 | O   | LEU | 195 | 46.823 | -4.525  | 3.303  | 1.00 | 0.00 | 3A4 |
| ATOM | 1153 | N   | ASN | 196 | 46.462 | -5.133  | 5.522  | 1.00 | 0.00 | 3A4 |
| ATOM | 1154 | CA  | ASN | 196 | 46.660 | -6.447  | 5.007  | 1.00 | 0.00 | 3A4 |
| ATOM | 1155 | CB  | ASN | 196 | 48.141 | -6.561  | 4.645  | 1.00 | 0.00 | 3A4 |
| ATOM | 1156 | CG  | ASN | 196 | 48.532 | -7.677  | 3.641  | 1.00 | 0.00 | 3A4 |
| ATOM | 1157 | OD1 | ASN | 196 | 49.287 | -8.581  | 3.992  | 1.00 | 0.00 | 3A4 |
| ATOM | 1158 | ND2 | ASN | 196 | 48.039 | -7.601  | 2.374  | 1.00 | 0.00 | 3A4 |
| ATOM | 1159 | C   | ASN | 196 | 46.000 | -7.578  | 5.603  | 1.00 | 0.00 | 3A4 |
| ATOM | 1160 | O   | ASN | 196 | 44.826 | -7.879  | 5.338  | 1.00 | 0.00 | 3A4 |
| ATOM | 1161 | N   | ASN | 197 | 46.757 | -8.297  | 6.407  | 1.00 | 0.00 | 3A4 |
| ATOM | 1162 | CA  | ASN | 197 | 46.317 | -9.599  | 6.859  | 1.00 | 0.00 | 3A4 |
| ATOM | 1163 | CB  | ASN | 197 | 47.456 | -10.511 | 7.443  | 1.00 | 0.00 | 3A4 |
| ATOM | 1164 | CG  | ASN | 197 | 48.572 | -10.689 | 6.405  | 1.00 | 0.00 | 3A4 |
| ATOM | 1165 | OD1 | ASN | 197 | 48.334 | -11.249 | 5.336  | 1.00 | 0.00 | 3A4 |
| ATOM | 1166 | ND2 | ASN | 197 | 49.810 | -10.219 | 6.717  | 1.00 | 0.00 | 3A4 |
| ATOM | 1167 | C   | ASN | 197 | 45.160 | -9.556  | 7.804  | 1.00 | 0.00 | 3A4 |
| ATOM | 1168 | O   | ASN | 197 | 44.307 | -10.439 | 7.761  | 1.00 | 0.00 | 3A4 |
| ATOM | 1169 | N   | PRO | 198 | 45.075 | -8.496  | 8.595  | 1.00 | 0.00 | 3A4 |
| ATOM | 1170 | CA  | PRO | 198 | 44.013 | -8.420  | 9.555  | 1.00 | 0.00 | 3A4 |
| ATOM | 1171 | CD  | PRO | 198 | 46.277 | -7.818  | 9.154  | 1.00 | 0.00 | 3A4 |
| ATOM | 1172 | CB  | PRO | 198 | 44.652 | -7.631  | 10.641 | 1.00 | 0.00 | 3A4 |
| ATOM | 1173 | CG  | PRO | 198 | 46.123 | -7.908  | 10.628 | 1.00 | 0.00 | 3A4 |
| ATOM | 1174 | C   | PRO | 198 | 42.754 | -7.786  | 9.085  | 1.00 | 0.00 | 3A4 |
| ATOM | 1175 | O   | PRO | 198 | 41.799 | -7.743  | 9.865  | 1.00 | 0.00 | 3A4 |
| ATOM | 1176 | N   | GLN | 199 | 42.701 | -7.279  | 7.830  | 1.00 | 0.00 | 3A4 |
| ATOM | 1177 | CA  | GLN | 199 | 41.636 | -6.407  | 7.407  | 1.00 | 0.00 | 3A4 |
| ATOM | 1178 | CB  | GLN | 199 | 41.900 | -5.668  | 6.066  | 1.00 | 0.00 | 3A4 |
| ATOM | 1179 | CG  | GLN | 199 | 41.001 | -4.419  | 5.844  | 1.00 | 0.00 | 3A4 |
| ATOM | 1180 | CD  | GLN | 199 | 41.471 | -3.266  | 6.742  | 1.00 | 0.00 | 3A4 |
| ATOM | 1181 | OE1 | GLN | 199 | 42.353 | -2.503  | 6.348  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1182 | NE2 | GLN | 199 | 40.885 | -3.125  | 7.963  | 1.00 | 0.00 | 3A4 |
| ATOM | 1183 | C   | GLN | 199 | 40.319 | -7.071  | 7.338  | 1.00 | 0.00 | 3A4 |
| ATOM | 1184 | O   | GLN | 199 | 39.374 | -6.533  | 7.889  | 1.00 | 0.00 | 3A4 |
| ATOM | 1185 | N   | ASP | 200 | 40.193 | -8.262  | 6.717  | 1.00 | 0.00 | 3A4 |
| ATOM | 1186 | CA  | ASP | 200 | 38.939 | -8.983  | 6.597  | 1.00 | 0.00 | 3A4 |
| ATOM | 1187 | CB  | ASP | 200 | 39.049 | -10.138 | 5.538  | 1.00 | 0.00 | 3A4 |
| ATOM | 1188 | CG  | ASP | 200 | 37.683 | -10.693 | 5.079  | 1.00 | 0.00 | 3A4 |
| ATOM | 1189 | OD1 | ASP | 200 | 37.459 | -11.923 | 5.238  | 1.00 | 0.00 | 3A4 |
| ATOM | 1190 | OD2 | ASP | 200 | 36.855 | -9.893  | 4.566  | 1.00 | 0.00 | 3A4 |
| ATOM | 1191 | C   | ASP | 200 | 38.347 | -9.432  | 7.927  | 1.00 | 0.00 | 3A4 |
| ATOM | 1192 | O   | ASP | 200 | 37.137 | -9.315  | 8.099  | 1.00 | 0.00 | 3A4 |
| ATOM | 1193 | N   | PRO | 201 | 39.155 | -9.847  | 8.917  | 1.00 | 0.00 | 3A4 |
| ATOM | 1194 | CA  | PRO | 201 | 38.699 | -10.088 | 10.270 | 1.00 | 0.00 | 3A4 |
| ATOM | 1195 | CD  | PRO | 201 | 40.343 | -10.678 | 8.654  | 1.00 | 0.00 | 3A4 |
| ATOM | 1196 | CB  | PRO | 201 | 39.936 | -10.637 | 11.012 | 1.00 | 0.00 | 3A4 |
| ATOM | 1197 | CG  | PRO | 201 | 40.633 | -11.466 | 9.938  | 1.00 | 0.00 | 3A4 |
| ATOM | 1198 | C   | PRO | 201 | 38.128 | -8.916  | 10.997 | 1.00 | 0.00 | 3A4 |
| ATOM | 1199 | O   | PRO | 201 | 37.076 | -9.052  | 11.615 | 1.00 | 0.00 | 3A4 |
| ATOM | 1200 | N   | PHE | 202 | 38.762 | -7.733  | 10.872 | 1.00 | 0.00 | 3A4 |
| ATOM | 1201 | CA  | PHE | 202 | 38.319 | -6.521  | 11.530 | 1.00 | 0.00 | 3A4 |
| ATOM | 1202 | CB  | PHE | 202 | 39.462 | -5.473  | 11.494 | 1.00 | 0.00 | 3A4 |
| ATOM | 1203 | CG  | PHE | 202 | 40.009 | -5.259  | 12.888 | 1.00 | 0.00 | 3A4 |
| ATOM | 1204 | CD1 | PHE | 202 | 40.365 | -6.366  | 13.691 | 1.00 | 0.00 | 3A4 |
| ATOM | 1205 | CD2 | PHE | 202 | 40.293 | -3.968  | 13.372 | 1.00 | 0.00 | 3A4 |
| ATOM | 1206 | CE1 | PHE | 202 | 40.856 | -6.184  | 14.987 | 1.00 | 0.00 | 3A4 |
| ATOM | 1207 | CE2 | PHE | 202 | 40.855 | -3.790  | 14.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 1208 | CZ  | PHE | 202 | 41.107 | -4.894  | 15.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 1209 | C   | PHE | 202 | 37.080 | -5.964  | 10.887 | 1.00 | 0.00 | 3A4 |
| ATOM | 1210 | O   | PHE | 202 | 36.208 | -5.444  | 11.573 | 1.00 | 0.00 | 3A4 |
| ATOM | 1211 | N   | VAL | 203 | 36.928 | -6.145  | 9.554  | 1.00 | 0.00 | 3A4 |
| ATOM | 1212 | CA  | VAL | 203 | 35.752 | -5.762  | 8.799  | 1.00 | 0.00 | 3A4 |
| ATOM | 1213 | CB  | VAL | 203 | 36.015 | -5.808  | 7.287  | 1.00 | 0.00 | 3A4 |
| ATOM | 1214 | CG1 | VAL | 203 | 34.738 | -5.677  | 6.411  | 1.00 | 0.00 | 3A4 |
| ATOM | 1215 | CG2 | VAL | 203 | 36.983 | -4.648  | 6.954  | 1.00 | 0.00 | 3A4 |
| ATOM | 1216 | C   | VAL | 203 | 34.545 | -6.596  | 9.199  | 1.00 | 0.00 | 3A4 |
| ATOM | 1217 | O   | VAL | 203 | 33.451 | -6.068  | 9.364  | 1.00 | 0.00 | 3A4 |
| ATOM | 1218 | N   | GLU | 204 | 34.736 | -7.908  | 9.475  | 1.00 | 0.00 | 3A4 |
| ATOM | 1219 | CA  | GLU | 204 | 33.684 | -8.782  | 9.967  | 1.00 | 0.00 | 3A4 |
| ATOM | 1220 | CB  | GLU | 204 | 34.114 | -10.262 | 9.912  | 1.00 | 0.00 | 3A4 |
| ATOM | 1221 | CG  | GLU | 204 | 34.199 | -10.797 | 8.472  | 1.00 | 0.00 | 3A4 |
| ATOM | 1222 | CD  | GLU | 204 | 34.793 | -12.210 | 8.489  | 1.00 | 0.00 | 3A4 |
| ATOM | 1223 | OE1 | GLU | 204 | 35.910 | -12.394 | 7.934  | 1.00 | 0.00 | 3A4 |
| ATOM | 1224 | OE2 | GLU | 204 | 34.137 | -13.123 | 9.059  | 1.00 | 0.00 | 3A4 |
| ATOM | 1225 | C   | GLU | 204 | 33.230 | -8.440  | 11.373 | 1.00 | 0.00 | 3A4 |
| ATOM | 1226 | O   | GLU | 204 | 32.042 | -8.449  | 11.666 | 1.00 | 0.00 | 3A4 |
| ATOM | 1227 | N   | ASN | 205 | 34.176 | -8.057  | 12.259 | 1.00 | 0.00 | 3A4 |
| ATOM | 1228 | CA  | ASN | 205 | 33.914 | -7.660  | 13.628 | 1.00 | 0.00 | 3A4 |
| ATOM | 1229 | CB  | ASN | 205 | 35.248 | -7.438  | 14.383 | 1.00 | 0.00 | 3A4 |
| ATOM | 1230 | CG  | ASN | 205 | 36.015 | -8.751  | 14.628 | 1.00 | 0.00 | 3A4 |
| ATOM | 1231 | OD1 | ASN | 205 | 37.233 | -8.776  | 14.460 | 1.00 | 0.00 | 3A4 |
| ATOM | 1232 | ND2 | ASN | 205 | 35.329 | -9.842  | 15.069 | 1.00 | 0.00 | 3A4 |
| ATOM | 1233 | C   | ASN | 205 | 33.087 | -6.395  | 13.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 1234 | O   | ASN | 205 | 32.115 | -6.344  | 14.487 | 1.00 | 0.00 | 3A4 |
| ATOM | 1235 | N   | THR | 206 | 33.414 | -5.376  | 12.903 | 1.00 | 0.00 | 3A4 |
| ATOM | 1236 | CA  | THR | 206 | 32.762 | -4.077  | 12.899 | 1.00 | 0.00 | 3A4 |
| ATOM | 1237 | CB  | THR | 206 | 33.525 | -3.007  | 12.102 | 1.00 | 0.00 | 3A4 |
| ATOM | 1238 | OG1 | THR | 206 | 34.406 | -3.549  | 11.139 | 1.00 | 0.00 | 3A4 |
| ATOM | 1239 | CG2 | THR | 206 | 34.381 | -2.246  | 13.141 | 1.00 | 0.00 | 3A4 |
| ATOM | 1240 | C   | THR | 206 | 31.364 | -4.178  | 12.322 | 1.00 | 0.00 | 3A4 |
| ATOM | 1241 | O   | THR | 206 | 30.435 | -3.581  | 12.843 | 1.00 | 0.00 | 3A4 |
| ATOM | 1242 | N   | LYS | 207 | 31.178 | -5.009  | 11.279 | 1.00 | 0.00 | 3A4 |
| ATOM | 1243 | CA  | LYS | 207 | 29.905 | -5.266  | 10.645 | 1.00 | 0.00 | 3A4 |
| ATOM | 1244 | CB  | LYS | 207 | 30.122 | -6.061  | 9.349  | 1.00 | 0.00 | 3A4 |
| ATOM | 1245 | CG  | LYS | 207 | 28.927 | -6.211  | 8.393  | 1.00 | 0.00 | 3A4 |
| ATOM | 1246 | CD  | LYS | 207 | 29.306 | -6.802  | 7.027  | 1.00 | 0.00 | 3A4 |
| ATOM | 1247 | CE  | LYS | 207 | 29.832 | -8.246  | 7.088  | 1.00 | 0.00 | 3A4 |
| ATOM | 1248 | NZ  | LYS | 207 | 30.150 | -8.750  | 5.731  | 1.00 | 0.00 | 3A4 |
| ATOM | 1249 | C   | LYS | 207 | 28.938 | -6.023  | 11.523 | 1.00 | 0.00 | 3A4 |
| ATOM | 1250 | O   | LYS | 207 | 27.753 | -5.736  | 11.533 | 1.00 | 0.00 | 3A4 |
| ATOM | 1251 | N   | LYS | 208 | 29.441 | -6.958  | 12.359 | 1.00 | 0.00 | 3A4 |
| ATOM | 1252 | CA  | LYS | 208 | 28.646 | -7.727  | 13.293 | 1.00 | 0.00 | 3A4 |
| ATOM | 1253 | CB  | LYS | 208 | 29.443 | -8.920  | 13.865 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1254 | CG  | LYS | 208 | 28.627 | -9.993  | 14.610 | 1.00 | 0.00 | 3A4 |
| ATOM | 1255 | CD  | LYS | 208 | 29.414 | -11.248 | 15.031 | 1.00 | 0.00 | 3A4 |
| ATOM | 1256 | CE  | LYS | 208 | 29.894 | -12.177 | 13.900 | 1.00 | 0.00 | 3A4 |
| ATOM | 1257 | NZ  | LYS | 208 | 31.125 | -11.677 | 13.236 | 1.00 | 0.00 | 3A4 |
| ATOM | 1258 | C   | LYS | 208 | 28.094 | -6.905  | 14.430 | 1.00 | 0.00 | 3A4 |
| ATOM | 1259 | O   | LYS | 208 | 26.931 | -7.047  | 14.780 | 1.00 | 0.00 | 3A4 |
| ATOM | 1260 | N   | LEU | 209 | 28.886 | -5.983  | 15.022 | 1.00 | 0.00 | 3A4 |
| ATOM | 1261 | CA  | LEU | 209 | 28.454 | -5.149  | 16.133 | 1.00 | 0.00 | 3A4 |
| ATOM | 1262 | CB  | LEU | 209 | 29.656 | -4.415  | 16.784 | 1.00 | 0.00 | 3A4 |
| ATOM | 1263 | CG  | LEU | 209 | 29.353 | -3.397  | 17.945 | 1.00 | 0.00 | 3A4 |
| ATOM | 1264 | CD1 | LEU | 209 | 28.592 | -4.009  | 19.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 1265 | CD2 | LEU | 209 | 30.596 | -2.606  | 18.399 | 1.00 | 0.00 | 3A4 |
| ATOM | 1266 | C   | LEU | 209 | 27.416 | -4.112  | 15.737 | 1.00 | 0.00 | 3A4 |
| ATOM | 1267 | O   | LEU | 209 | 26.515 | -3.793  | 16.507 | 1.00 | 0.00 | 3A4 |
| ATOM | 1268 | N   | LEU | 210 | 27.527 | -3.561  | 14.510 | 1.00 | 0.00 | 3A4 |
| ATOM | 1269 | CA  | LEU | 210 | 26.707 | -2.449  | 14.080 | 1.00 | 0.00 | 3A4 |
| ATOM | 1270 | CB  | LEU | 210 | 27.559 | -1.343  | 13.418 | 1.00 | 0.00 | 3A4 |
| ATOM | 1271 | CG  | LEU | 210 | 28.684 | -0.850  | 14.384 | 1.00 | 0.00 | 3A4 |
| ATOM | 1272 | CD1 | LEU | 210 | 29.655 | 0.113   | 13.699 | 1.00 | 0.00 | 3A4 |
| ATOM | 1273 | CD2 | LEU | 210 | 28.176 | -0.257  | 15.717 | 1.00 | 0.00 | 3A4 |
| ATOM | 1274 | C   | LEU | 210 | 25.611 | -2.862  | 13.145 | 1.00 | 0.00 | 3A4 |
| ATOM | 1275 | O   | LEU | 210 | 24.465 | -2.454  | 13.335 | 1.00 | 0.00 | 3A4 |
| ATOM | 1276 | N   | ARG | 211 | 25.948 | -3.571  | 12.035 | 1.00 | 0.00 | 3A4 |
| ATOM | 1277 | CA  | ARG | 211 | 25.146 | -3.650  | 10.816 | 1.00 | 0.00 | 3A4 |
| ATOM | 1278 | CB  | ARG | 211 | 26.033 | -3.592  | 9.539  | 1.00 | 0.00 | 3A4 |
| ATOM | 1279 | CG  | ARG | 211 | 26.927 | -2.337  | 9.503  | 1.00 | 0.00 | 3A4 |
| ATOM | 1280 | CD  | ARG | 211 | 27.841 | -2.220  | 8.274  | 1.00 | 0.00 | 3A4 |
| ATOM | 1281 | NE  | ARG | 211 | 27.005 | -2.107  | 7.024  | 1.00 | 0.00 | 3A4 |
| ATOM | 1282 | CZ  | ARG | 211 | 26.814 | -0.939  | 6.329  | 1.00 | 0.00 | 3A4 |
| ATOM | 1283 | NH1 | ARG | 211 | 26.014 | -0.951  | 5.223  | 1.00 | 0.00 | 3A4 |
| ATOM | 1284 | NH2 | ARG | 211 | 27.397 | 0.236   | 6.711  | 1.00 | 0.00 | 3A4 |
| ATOM | 1285 | C   | ARG | 211 | 24.236 | -4.864  | 10.757 | 1.00 | 0.00 | 3A4 |
| ATOM | 1286 | O   | ARG | 211 | 23.275 | -4.868  | 9.989  | 1.00 | 0.00 | 3A4 |
| ATOM | 1287 | N   | PHE | 212 | 24.496 | -5.910  | 11.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 1288 | CA  | PHE | 212 | 23.555 | -6.992  | 11.826 | 1.00 | 0.00 | 3A4 |
| ATOM | 1289 | CB  | PHE | 212 | 23.730 | -8.273  | 10.930 | 1.00 | 0.00 | 3A4 |
| ATOM | 1290 | CG  | PHE | 212 | 25.061 | -8.998  | 10.978 | 1.00 | 0.00 | 3A4 |
| ATOM | 1291 | CD1 | PHE | 212 | 25.170 | -10.224 | 11.667 | 1.00 | 0.00 | 3A4 |
| ATOM | 1292 | CD2 | PHE | 212 | 26.182 | -8.527  | 10.268 | 1.00 | 0.00 | 3A4 |
| ATOM | 1293 | CE1 | PHE | 212 | 26.367 | -10.954 | 11.660 | 1.00 | 0.00 | 3A4 |
| ATOM | 1294 | CE2 | PHE | 212 | 27.380 | -9.259  | 10.254 | 1.00 | 0.00 | 3A4 |
| ATOM | 1295 | CZ  | PHE | 212 | 27.474 | -10.469 | 10.952 | 1.00 | 0.00 | 3A4 |
| ATOM | 1296 | C   | PHE | 212 | 23.608 | -7.246  | 13.314 | 1.00 | 0.00 | 3A4 |
| ATOM | 1297 | O   | PHE | 212 | 24.292 | -8.143  | 13.802 | 1.00 | 0.00 | 3A4 |
| ATOM | 1298 | N   | ASP | 213 | 22.863 | -6.398  | 14.068 | 1.00 | 0.00 | 3A4 |
| ATOM | 1299 | CA  | ASP | 213 | 22.843 | -6.356  | 15.513 | 1.00 | 0.00 | 3A4 |
| ATOM | 1300 | CB  | ASP | 213 | 23.642 | -5.131  | 16.046 | 1.00 | 0.00 | 3A4 |
| ATOM | 1301 | CG  | ASP | 213 | 23.916 | -5.215  | 17.558 | 1.00 | 0.00 | 3A4 |
| ATOM | 1302 | OD1 | ASP | 213 | 24.608 | -6.179  | 17.982 | 1.00 | 0.00 | 3A4 |
| ATOM | 1303 | OD2 | ASP | 213 | 23.444 | -4.312  | 18.300 | 1.00 | 0.00 | 3A4 |
| ATOM | 1304 | C   | ASP | 213 | 21.391 | -6.281  | 15.902 | 1.00 | 0.00 | 3A4 |
| ATOM | 1305 | O   | ASP | 213 | 20.714 | -5.286  | 15.648 | 1.00 | 0.00 | 3A4 |
| ATOM | 1306 | N   | PHE | 214 | 20.894 | -7.371  | 16.533 | 1.00 | 0.00 | 3A4 |
| ATOM | 1307 | CA  | PHE | 214 | 19.516 | -7.516  | 16.941 | 1.00 | 0.00 | 3A4 |
| ATOM | 1308 | CB  | PHE | 214 | 18.526 | -7.900  | 15.776 | 1.00 | 0.00 | 3A4 |
| ATOM | 1309 | CG  | PHE | 214 | 19.127 | -8.826  | 14.734 | 1.00 | 0.00 | 3A4 |
| ATOM | 1310 | CD1 | PHE | 214 | 19.610 | -8.306  | 13.515 | 1.00 | 0.00 | 3A4 |
| ATOM | 1311 | CD2 | PHE | 214 | 19.216 | -10.215 | 14.950 | 1.00 | 0.00 | 3A4 |
| ATOM | 1312 | CE1 | PHE | 214 | 20.186 | -9.143  | 12.550 | 1.00 | 0.00 | 3A4 |
| ATOM | 1313 | CE2 | PHE | 214 | 19.793 | -11.058 | 13.987 | 1.00 | 0.00 | 3A4 |
| ATOM | 1314 | CZ  | PHE | 214 | 20.280 | -10.520 | 12.788 | 1.00 | 0.00 | 3A4 |
| ATOM | 1315 | C   | PHE | 214 | 19.513 | -8.554  | 18.034 | 1.00 | 0.00 | 3A4 |
| ATOM | 1316 | O   | PHE | 214 | 20.344 | -9.460  | 18.058 | 1.00 | 0.00 | 3A4 |
| ATOM | 1317 | N   | LEU | 215 | 18.527 | -8.428  | 18.956 | 1.00 | 0.00 | 3A4 |
| ATOM | 1318 | CA  | LEU | 215 | 18.216 | -9.384  | 19.995 | 1.00 | 0.00 | 3A4 |
| ATOM | 1319 | CB  | LEU | 215 | 18.914 | -9.072  | 21.353 | 1.00 | 0.00 | 3A4 |
| ATOM | 1320 | CG  | LEU | 215 | 18.685 | -10.089 | 22.505 | 1.00 | 0.00 | 3A4 |
| ATOM | 1321 | CD1 | LEU | 215 | 19.075 | -11.533 | 22.128 | 1.00 | 0.00 | 3A4 |
| ATOM | 1322 | CD2 | LEU | 215 | 19.419 | -9.639  | 23.783 | 1.00 | 0.00 | 3A4 |
| ATOM | 1323 | C   | LEU | 215 | 16.716 | -9.298  | 20.078 | 1.00 | 0.00 | 3A4 |
| ATOM | 1324 | O   | LEU | 215 | 16.151 | -8.667  | 20.970 | 1.00 | 0.00 | 3A4 |
| ATOM | 1325 | N   | ASP | 216 | 16.046 | -9.926  | 19.073 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1326 | CA  | ASP | 216 | 14.627 | -9.830  | 18.781 | 1.00 | 0.00 | 3A4 |
| ATOM | 1327 | CB  | ASP | 216 | 14.369 | -9.623  | 17.242 | 1.00 | 0.00 | 3A4 |
| ATOM | 1328 | CG  | ASP | 216 | 14.915 | -10.746 | 16.328 | 1.00 | 0.00 | 3A4 |
| ATOM | 1329 | OD1 | ASP | 216 | 16.161 | -10.914 | 16.241 | 1.00 | 0.00 | 3A4 |
| ATOM | 1330 | OD2 | ASP | 216 | 14.075 | -11.445 | 15.700 | 1.00 | 0.00 | 3A4 |
| ATOM | 1331 | C   | ASP | 216 | 13.914 | -11.069 | 19.316 | 1.00 | 0.00 | 3A4 |
| ATOM | 1332 | O   | ASP | 216 | 14.578 | -12.088 | 19.506 | 1.00 | 0.00 | 3A4 |
| ATOM | 1333 | N   | PRO | 217 | 12.576 | -11.062 | 19.553 | 1.00 | 0.00 | 3A4 |
| ATOM | 1334 | CA  | PRO | 217 | 11.794 | -12.227 | 19.974 | 1.00 | 0.00 | 3A4 |
| ATOM | 1335 | CD  | PRO | 217 | 11.814 | -9.819  | 19.695 | 1.00 | 0.00 | 3A4 |
| ATOM | 1336 | CB  | PRO | 217 | 10.525 | -11.614 | 20.611 | 1.00 | 0.00 | 3A4 |
| ATOM | 1337 | CG  | PRO | 217 | 10.367 | -10.231 | 19.970 | 1.00 | 0.00 | 3A4 |
| ATOM | 1338 | C   | PRO | 217 | 11.504 | -13.148 | 18.786 | 1.00 | 0.00 | 3A4 |
| ATOM | 1339 | O   | PRO | 217 | 12.309 | -14.043 | 18.527 | 1.00 | 0.00 | 3A4 |
| ATOM | 1340 | N   | PHE | 218 | 10.374 | -12.933 | 18.064 | 1.00 | 0.00 | 3A4 |
| ATOM | 1341 | CA  | PHE | 218 | 10.004 | -13.621 | 16.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 1342 | CB  | PHE | 218 | 8.877  | -14.691 | 17.032 | 1.00 | 0.00 | 3A4 |
| ATOM | 1343 | CG  | PHE | 218 | 9.294  | -15.734 | 18.036 | 1.00 | 0.00 | 3A4 |
| ATOM | 1344 | CD1 | PHE | 218 | 8.630  | -15.831 | 19.273 | 1.00 | 0.00 | 3A4 |
| ATOM | 1345 | CD2 | PHE | 218 | 10.354 | -16.621 | 17.766 | 1.00 | 0.00 | 3A4 |
| ATOM | 1346 | CE1 | PHE | 218 | 9.018  | -16.783 | 20.225 | 1.00 | 0.00 | 3A4 |
| ATOM | 1347 | CE2 | PHE | 218 | 10.751 | -17.572 | 18.720 | 1.00 | 0.00 | 3A4 |
| ATOM | 1348 | CZ  | PHE | 218 | 10.083 | -17.651 | 19.950 | 1.00 | 0.00 | 3A4 |
| ATOM | 1349 | C   | PHE | 218 | 9.495  | -12.564 | 15.883 | 1.00 | 0.00 | 3A4 |
| ATOM | 1350 | O   | PHE | 218 | 9.158  | -12.860 | 14.737 | 1.00 | 0.00 | 3A4 |
| ATOM | 1351 | N   | PHE | 219 | 9.400  | -11.297 | 16.374 | 1.00 | 0.00 | 3A4 |
| ATOM | 1352 | CA  | PHE | 219 | 8.762  | -10.165 | 15.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 1353 | CB  | PHE | 219 | 7.558  | -9.630  | 16.572 | 1.00 | 0.00 | 3A4 |
| ATOM | 1354 | CG  | PHE | 219 | 6.443  | -10.646 | 16.570 | 1.00 | 0.00 | 3A4 |
| ATOM | 1355 | CD1 | PHE | 219 | 5.437  | -10.600 | 15.587 | 1.00 | 0.00 | 3A4 |
| ATOM | 1356 | CD2 | PHE | 219 | 6.389  | -11.664 | 17.542 | 1.00 | 0.00 | 3A4 |
| ATOM | 1357 | CE1 | PHE | 219 | 4.401  | -11.546 | 15.576 | 1.00 | 0.00 | 3A4 |
| ATOM | 1358 | CE2 | PHE | 219 | 5.356  | -12.611 | 17.536 | 1.00 | 0.00 | 3A4 |
| ATOM | 1359 | CZ  | PHE | 219 | 4.360  | -12.551 | 16.553 | 1.00 | 0.00 | 3A4 |
| ATOM | 1360 | C   | PHE | 219 | 9.798  | -9.078  | 15.602 | 1.00 | 0.00 | 3A4 |
| ATOM | 1361 | O   | PHE | 219 | 10.805 | -9.068  | 16.307 | 1.00 | 0.00 | 3A4 |
| ATOM | 1362 | N   | LEU | 220 | 9.547  | -8.131  | 14.664 | 1.00 | 0.00 | 3A4 |
| ATOM | 1363 | CA  | LEU | 220 | 10.447 | -7.050  | 14.321 | 1.00 | 0.00 | 3A4 |
| ATOM | 1364 | CB  | LEU | 220 | 11.550 | -7.452  | 13.279 | 1.00 | 0.00 | 3A4 |
| ATOM | 1365 | CG  | LEU | 220 | 11.130 | -7.889  | 11.840 | 1.00 | 0.00 | 3A4 |
| ATOM | 1366 | CD1 | LEU | 220 | 12.368 | -7.938  | 10.924 | 1.00 | 0.00 | 3A4 |
| ATOM | 1367 | CD2 | LEU | 220 | 10.365 | -9.229  | 11.764 | 1.00 | 0.00 | 3A4 |
| ATOM | 1368 | C   | LEU | 220 | 9.590  | -5.908  | 13.825 | 1.00 | 0.00 | 3A4 |
| ATOM | 1369 | O   | LEU | 220 | 8.366  | -5.964  | 13.937 | 1.00 | 0.00 | 3A4 |
| ATOM | 1370 | N   | SER | 221 | 10.268 | -4.849  | 13.284 | 1.00 | 0.00 | 3A4 |
| ATOM | 1371 | CA  | SER | 221 | 9.781  | -3.584  | 12.735 | 1.00 | 0.00 | 3A4 |
| ATOM | 1372 | CB  | SER | 221 | 8.270  | -3.542  | 12.288 | 1.00 | 0.00 | 3A4 |
| ATOM | 1373 | OG  | SER | 221 | 7.980  | -2.485  | 11.376 | 1.00 | 0.00 | 3A4 |
| ATOM | 1374 | C   | SER | 221 | 10.129 | -2.514  | 13.764 | 1.00 | 0.00 | 3A4 |
| ATOM | 1375 | O   | SER | 221 | 10.958 | -2.740  | 14.646 | 1.00 | 0.00 | 3A4 |
| ATOM | 1376 | N   | ILE | 222 | 9.495  | -1.312  | 13.661 | 1.00 | 0.00 | 3A4 |
| ATOM | 1377 | CA  | ILE | 222 | 9.692  | -0.155  | 14.524 | 1.00 | 0.00 | 3A4 |
| ATOM | 1378 | CB  | ILE | 222 | 9.886  | 1.145   | 13.735 | 1.00 | 0.00 | 3A4 |
| ATOM | 1379 | CG2 | ILE | 222 | 11.258 | 1.038   | 13.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 1380 | CG1 | ILE | 222 | 8.727  | 1.449   | 12.741 | 1.00 | 0.00 | 3A4 |
| ATOM | 1381 | CD  | ILE | 222 | 8.868  | 2.791   | 12.016 | 1.00 | 0.00 | 3A4 |
| ATOM | 1382 | C   | ILE | 222 | 8.533  | -0.038  | 15.500 | 1.00 | 0.00 | 3A4 |
| ATOM | 1383 | O   | ILE | 222 | 8.631  | 0.670   | 16.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 1384 | N   | THR | 223 | 7.406  | -0.746  | 15.215 | 1.00 | 0.00 | 3A4 |
| ATOM | 1385 | CA  | THR | 223 | 6.225  | -0.787  | 16.050 | 1.00 | 0.00 | 3A4 |
| ATOM | 1386 | CB  | THR | 223 | 5.259  | 0.384   | 15.782 | 1.00 | 0.00 | 3A4 |
| ATOM | 1387 | OG1 | THR | 223 | 4.159  | 0.414   | 16.691 | 1.00 | 0.00 | 3A4 |
| ATOM | 1388 | CG2 | THR | 223 | 4.751  | 0.459   | 14.318 | 1.00 | 0.00 | 3A4 |
| ATOM | 1389 | C   | THR | 223 | 5.633  | -2.165  | 15.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 1390 | O   | THR | 223 | 5.360  | -2.558  | 14.678 | 1.00 | 0.00 | 3A4 |
| ATOM | 1391 | N   | VAL | 224 | 5.435  | -2.927  | 16.918 | 1.00 | 0.00 | 3A4 |
| ATOM | 1392 | CA  | VAL | 224 | 4.832  | -4.244  | 16.917 | 1.00 | 0.00 | 3A4 |
| ATOM | 1393 | CB  | VAL | 224 | 5.751  | -5.354  | 16.379 | 1.00 | 0.00 | 3A4 |
| ATOM | 1394 | CG1 | VAL | 224 | 7.065  | -5.517  | 17.186 | 1.00 | 0.00 | 3A4 |
| ATOM | 1395 | CG2 | VAL | 224 | 4.973  | -6.679  | 16.198 | 1.00 | 0.00 | 3A4 |
| ATOM | 1396 | C   | VAL | 224 | 4.397  | -4.468  | 18.349 | 1.00 | 0.00 | 3A4 |
| ATOM | 1397 | O   | VAL | 224 | 5.085  | -4.071  | 19.290 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1398 | N   | PHE | 225 | 3.212  | -5.114  | 18.534 | 1.00 | 0.00 | 3A4 |
| ATOM | 1399 | CA  | PHE | 225 | 2.568  | -5.398  | 19.809 | 1.00 | 0.00 | 3A4 |
| ATOM | 1400 | CB  | PHE | 225 | 1.025  | -5.112  | 19.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 1401 | CG  | PHE | 225 | 0.345  | -5.089  | 21.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 1402 | CD1 | PHE | 225 | 0.584  | -4.036  | 21.993 | 1.00 | 0.00 | 3A4 |
| ATOM | 1403 | CD2 | PHE | 225 | -0.533 | -6.123  | 21.470 | 1.00 | 0.00 | 3A4 |
| ATOM | 1404 | CE1 | PHE | 225 | -0.038 | -4.017  | 23.251 | 1.00 | 0.00 | 3A4 |
| ATOM | 1405 | CE2 | PHE | 225 | -1.156 | -6.107  | 22.726 | 1.00 | 0.00 | 3A4 |
| ATOM | 1406 | CZ  | PHE | 225 | -0.908 | -5.053  | 23.617 | 1.00 | 0.00 | 3A4 |
| ATOM | 1407 | C   | PHE | 225 | 2.898  | -6.812  | 20.313 | 1.00 | 0.00 | 3A4 |
| ATOM | 1408 | O   | PHE | 225 | 3.306  | -6.885  | 21.472 | 1.00 | 0.00 | 3A4 |
| ATOM | 1409 | N   | PRO | 226 | 2.776  | -7.964  | 19.590 | 1.00 | 0.00 | 3A4 |
| ATOM | 1410 | CA  | PRO | 226 | 3.087  | -9.298  | 20.117 | 1.00 | 0.00 | 3A4 |
| ATOM | 1411 | CD  | PRO | 226 | 2.027  | -8.062  | 18.335 | 1.00 | 0.00 | 3A4 |
| ATOM | 1412 | CB  | PRO | 226 | 2.324  | -10.268 | 19.186 | 1.00 | 0.00 | 3A4 |
| ATOM | 1413 | CG  | PRO | 226 | 2.191  | -9.507  | 17.865 | 1.00 | 0.00 | 3A4 |
| ATOM | 1414 | C   | PRO | 226 | 4.587  | -9.598  | 20.127 | 1.00 | 0.00 | 3A4 |
| ATOM | 1415 | O   | PRO | 226 | 5.346  | -9.003  | 19.361 | 1.00 | 0.00 | 3A4 |
| ATOM | 1416 | N   | PHE | 227 | 4.993  | -10.544 | 21.009 | 1.00 | 0.00 | 3A4 |
| ATOM | 1417 | CA  | PHE | 227 | 6.356  | -10.995 | 21.212 | 1.00 | 0.00 | 3A4 |
| ATOM | 1418 | CB  | PHE | 227 | 7.106  | -10.254 | 22.376 | 1.00 | 0.00 | 3A4 |
| ATOM | 1419 | CG  | PHE | 227 | 6.298  | -10.129 | 23.651 | 1.00 | 0.00 | 3A4 |
| ATOM | 1420 | CD1 | PHE | 227 | 5.437  | -9.031  | 23.855 | 1.00 | 0.00 | 3A4 |
| ATOM | 1421 | CD2 | PHE | 227 | 6.393  | -11.105 | 24.663 | 1.00 | 0.00 | 3A4 |
| ATOM | 1422 | CE1 | PHE | 227 | 4.677  | -8.920  | 25.028 | 1.00 | 0.00 | 3A4 |
| ATOM | 1423 | CE2 | PHE | 227 | 5.634  | -10.999 | 25.838 | 1.00 | 0.00 | 3A4 |
| ATOM | 1424 | CZ  | PHE | 227 | 4.775  | -9.907  | 26.019 | 1.00 | 0.00 | 3A4 |
| ATOM | 1425 | C   | PHE | 227 | 6.307  | -12.495 | 21.429 | 1.00 | 0.00 | 3A4 |
| ATOM | 1426 | O   | PHE | 227 | 7.291  | -13.188 | 21.177 | 1.00 | 0.00 | 3A4 |
| ATOM | 1427 | N   | LEU | 228 | 5.134  | -13.001 | 21.925 | 1.00 | 0.00 | 3A4 |
| ATOM | 1428 | CA  | LEU | 228 | 4.753  | -14.389 | 22.186 | 1.00 | 0.00 | 3A4 |
| ATOM | 1429 | CB  | LEU | 228 | 5.137  | -15.381 | 21.024 | 1.00 | 0.00 | 3A4 |
| ATOM | 1430 | CG  | LEU | 228 | 4.217  | -16.607 | 20.757 | 1.00 | 0.00 | 3A4 |
| ATOM | 1431 | CD1 | LEU | 228 | 4.267  | -17.707 | 21.832 | 1.00 | 0.00 | 3A4 |
| ATOM | 1432 | CD2 | LEU | 228 | 2.767  | -16.215 | 20.406 | 1.00 | 0.00 | 3A4 |
| ATOM | 1433 | C   | LEU | 228 | 5.274  | -14.788 | 23.565 | 1.00 | 0.00 | 3A4 |
| ATOM | 1434 | O   | LEU | 228 | 4.778  | -14.291 | 24.575 | 1.00 | 0.00 | 3A4 |
| ATOM | 1435 | N   | ILE | 229 | 6.316  | -15.659 | 23.623 | 1.00 | 0.00 | 3A4 |
| ATOM | 1436 | CA  | ILE | 229 | 7.097  | -15.948 | 24.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 1437 | CB  | ILE | 229 | 6.457  | -16.944 | 25.799 | 1.00 | 0.00 | 3A4 |
| ATOM | 1438 | CG2 | ILE | 229 | 6.056  | -18.311 | 25.188 | 1.00 | 0.00 | 3A4 |
| ATOM | 1439 | CG1 | ILE | 229 | 7.185  | -17.043 | 27.173 | 1.00 | 0.00 | 3A4 |
| ATOM | 1440 | CD  | ILE | 229 | 8.372  | -18.014 | 27.278 | 1.00 | 0.00 | 3A4 |
| ATOM | 1441 | C   | ILE | 229 | 8.458  | -16.351 | 24.252 | 1.00 | 0.00 | 3A4 |
| ATOM | 1442 | O   | ILE | 229 | 8.631  | -17.503 | 23.857 | 1.00 | 0.00 | 3A4 |
| ATOM | 1443 | N   | PRO | 230 | 9.474  | -15.455 | 24.157 | 1.00 | 0.00 | 3A4 |
| ATOM | 1444 | CA  | PRO | 230 | 10.759 | -15.735 | 23.519 | 1.00 | 0.00 | 3A4 |
| ATOM | 1445 | CD  | PRO | 230 | 9.306  | -14.022 | 24.410 | 1.00 | 0.00 | 3A4 |
| ATOM | 1446 | CB  | PRO | 230 | 11.244 | -14.349 | 23.055 | 1.00 | 0.00 | 3A4 |
| ATOM | 1447 | CG  | PRO | 230 | 10.655 | -13.376 | 24.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 1448 | C   | PRO | 230 | 11.749 | -16.380 | 24.483 | 1.00 | 0.00 | 3A4 |
| ATOM | 1449 | O   | PRO | 230 | 11.509 | -16.422 | 25.691 | 1.00 | 0.00 | 3A4 |
| ATOM | 1450 | N   | ILE | 231 | 12.894 | -16.870 | 23.931 | 1.00 | 0.00 | 3A4 |
| ATOM | 1451 | CA  | ILE | 231 | 13.997 | -17.495 | 24.644 | 1.00 | 0.00 | 3A4 |
| ATOM | 1452 | CB  | ILE | 231 | 14.463 | -18.802 | 23.988 | 1.00 | 0.00 | 3A4 |
| ATOM | 1453 | CG2 | ILE | 231 | 15.554 | -19.489 | 24.852 | 1.00 | 0.00 | 3A4 |
| ATOM | 1454 | CG1 | ILE | 231 | 13.275 | -19.767 | 23.714 | 1.00 | 0.00 | 3A4 |
| ATOM | 1455 | CD  | ILE | 231 | 12.502 | -20.240 | 24.953 | 1.00 | 0.00 | 3A4 |
| ATOM | 1456 | C   | ILE | 231 | 15.116 | -16.473 | 24.709 | 1.00 | 0.00 | 3A4 |
| ATOM | 1457 | O   | ILE | 231 | 15.691 | -16.247 | 25.773 | 1.00 | 0.00 | 3A4 |
| ATOM | 1458 | N   | LEU | 232 | 15.428 | -15.844 | 23.533 | 1.00 | 0.00 | 3A4 |
| ATOM | 1459 | CA  | LEU | 232 | 16.397 | -14.778 | 23.277 | 1.00 | 0.00 | 3A4 |
| ATOM | 1460 | CB  | LEU | 232 | 16.312 | -13.552 | 24.250 | 1.00 | 0.00 | 3A4 |
| ATOM | 1461 | CG  | LEU | 232 | 14.944 | -12.824 | 24.269 | 1.00 | 0.00 | 3A4 |
| ATOM | 1462 | CD1 | LEU | 232 | 14.900 | -11.763 | 25.383 | 1.00 | 0.00 | 3A4 |
| ATOM | 1463 | CD2 | LEU | 232 | 14.567 | -12.203 | 22.908 | 1.00 | 0.00 | 3A4 |
| ATOM | 1464 | C   | LEU | 232 | 17.814 | -15.328 | 23.232 | 1.00 | 0.00 | 3A4 |
| ATOM | 1465 | O   | LEU | 232 | 18.606 | -15.133 | 24.154 | 1.00 | 0.00 | 3A4 |
| ATOM | 1466 | N   | GLU | 233 | 18.131 | -16.047 | 22.125 | 1.00 | 0.00 | 3A4 |
| ATOM | 1467 | CA  | GLU | 233 | 19.390 | -16.728 | 21.896 | 1.00 | 0.00 | 3A4 |
| ATOM | 1468 | CB  | GLU | 233 | 19.269 | -18.268 | 22.115 | 1.00 | 0.00 | 3A4 |
| ATOM | 1469 | CG  | GLU | 233 | 18.095 | -18.955 | 21.373 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1470 | CD  | GLU | 233 | 18.120 | -20.462 | 21.648 | 1.00 | 0.00 | 3A4 |
| ATOM | 1471 | OE1 | GLU | 233 | 19.140 | -21.114 | 21.295 | 1.00 | 0.00 | 3A4 |
| ATOM | 1472 | OE2 | GLU | 233 | 17.118 | -20.985 | 22.205 | 1.00 | 0.00 | 3A4 |
| ATOM | 1473 | C   | GLU | 233 | 19.828 | -16.395 | 20.489 | 1.00 | 0.00 | 3A4 |
| ATOM | 1474 | O   | GLU | 233 | 20.256 | -17.261 | 19.726 | 1.00 | 0.00 | 3A4 |
| ATOM | 1475 | N   | VAL | 234 | 19.734 | -15.088 | 20.125 | 1.00 | 0.00 | 3A4 |
| ATOM | 1476 | CA  | VAL | 234 | 20.053 | -14.558 | 18.815 | 1.00 | 0.00 | 3A4 |
| ATOM | 1477 | CB  | VAL | 234 | 18.792 | -14.275 | 17.987 | 1.00 | 0.00 | 3A4 |
| ATOM | 1478 | CG1 | VAL | 234 | 17.739 | -13.402 | 18.723 | 1.00 | 0.00 | 3A4 |
| ATOM | 1479 | CG2 | VAL | 234 | 19.142 | -13.768 | 16.568 | 1.00 | 0.00 | 3A4 |
| ATOM | 1480 | C   | VAL | 234 | 20.960 | -13.370 | 19.064 | 1.00 | 0.00 | 3A4 |
| ATOM | 1481 | O   | VAL | 234 | 20.563 | -12.209 | 18.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 1482 | N   | LEU | 235 | 22.242 | -13.673 | 19.393 | 1.00 | 0.00 | 3A4 |
| ATOM | 1483 | CA  | LEU | 235 | 23.270 | -12.694 | 19.675 | 1.00 | 0.00 | 3A4 |
| ATOM | 1484 | CB  | LEU | 235 | 23.137 | -11.954 | 21.056 | 1.00 | 0.00 | 3A4 |
| ATOM | 1485 | CG  | LEU | 235 | 23.294 | -12.749 | 22.393 | 1.00 | 0.00 | 3A4 |
| ATOM | 1486 | CD1 | LEU | 235 | 23.236 | -11.785 | 23.594 | 1.00 | 0.00 | 3A4 |
| ATOM | 1487 | CD2 | LEU | 235 | 22.289 | -13.903 | 22.600 | 1.00 | 0.00 | 3A4 |
| ATOM | 1488 | C   | LEU | 235 | 24.592 | -13.413 | 19.593 | 1.00 | 0.00 | 3A4 |
| ATOM | 1489 | O   | LEU | 235 | 24.703 | -14.586 | 19.948 | 1.00 | 0.00 | 3A4 |
| ATOM | 1490 | N   | ASN | 236 | 25.638 | -12.684 | 19.128 | 1.00 | 0.00 | 3A4 |
| ATOM | 1491 | CA  | ASN | 236 | 27.013 | -13.135 | 19.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 1492 | CB  | ASN | 236 | 27.351 | -13.966 | 17.803 | 1.00 | 0.00 | 3A4 |
| ATOM | 1493 | CG  | ASN | 236 | 28.697 | -14.706 | 17.931 | 1.00 | 0.00 | 3A4 |
| ATOM | 1494 | OD1 | ASN | 236 | 28.818 | -15.613 | 18.753 | 1.00 | 0.00 | 3A4 |
| ATOM | 1495 | ND2 | ASN | 236 | 29.719 | -14.326 | 17.115 | 1.00 | 0.00 | 3A4 |
| ATOM | 1496 | C   | ASN | 236 | 27.795 | -11.845 | 19.165 | 1.00 | 0.00 | 3A4 |
| ATOM | 1497 | O   | ASN | 236 | 28.546 | -11.489 | 18.259 | 1.00 | 0.00 | 3A4 |
| ATOM | 1498 | N   | ILE | 237 | 27.590 | -11.096 | 20.283 | 1.00 | 0.00 | 3A4 |
| ATOM | 1499 | CA  | ILE | 237 | 28.074 | -9.747  | 20.504 | 1.00 | 0.00 | 3A4 |
| ATOM | 1500 | CB  | ILE | 237 | 26.980 | -8.800  | 20.998 | 1.00 | 0.00 | 3A4 |
| ATOM | 1501 | CG2 | ILE | 237 | 26.039 | -8.584  | 19.789 | 1.00 | 0.00 | 3A4 |
| ATOM | 1502 | CG1 | ILE | 237 | 26.203 | -9.271  | 22.262 | 1.00 | 0.00 | 3A4 |
| ATOM | 1503 | CD  | ILE | 237 | 25.059 | -8.341  | 22.671 | 1.00 | 0.00 | 3A4 |
| ATOM | 1504 | C   | ILE | 237 | 29.228 | -9.798  | 21.461 | 1.00 | 0.00 | 3A4 |
| ATOM | 1505 | O   | ILE | 237 | 30.202 | -9.126  | 21.226 | 1.00 | 0.00 | 3A4 |
| ATOM | 1506 | N   | CYS | 238 | 29.124 | -10.614 | 22.532 | 1.00 | 0.00 | 3A4 |
| ATOM | 1507 | CA  | CYS | 238 | 30.099 | -10.834 | 23.576 | 1.00 | 0.00 | 3A4 |
| ATOM | 1508 | CB  | CYS | 238 | 29.513 | -11.689 | 24.739 | 1.00 | 0.00 | 3A4 |
| ATOM | 1509 | SG  | CYS | 238 | 28.106 | -10.870 | 25.526 | 1.00 | 0.00 | 3A4 |
| ATOM | 1510 | C   | CYS | 238 | 31.307 | -11.563 | 23.083 | 1.00 | 0.00 | 3A4 |
| ATOM | 1511 | O   | CYS | 238 | 32.424 | -11.278 | 23.493 | 1.00 | 0.00 | 3A4 |
| ATOM | 1512 | N   | VAL | 239 | 31.138 | -12.446 | 22.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 1513 | CA  | VAL | 239 | 32.219 | -13.161 | 21.438 | 1.00 | 0.00 | 3A4 |
| ATOM | 1514 | CB  | VAL | 239 | 31.700 | -14.367 | 20.675 | 1.00 | 0.00 | 3A4 |
| ATOM | 1515 | CG1 | VAL | 239 | 32.858 | -15.308 | 20.247 | 1.00 | 0.00 | 3A4 |
| ATOM | 1516 | CG2 | VAL | 239 | 30.715 | -15.139 | 21.586 | 1.00 | 0.00 | 3A4 |
| ATOM | 1517 | C   | VAL | 239 | 33.006 | -12.283 | 20.505 | 1.00 | 0.00 | 3A4 |
| ATOM | 1518 | O   | VAL | 239 | 34.228 | -12.327 | 20.485 | 1.00 | 0.00 | 3A4 |
| ATOM | 1519 | N   | PHE | 240 | 32.315 | -11.420 | 19.731 | 1.00 | 0.00 | 3A4 |
| ATOM | 1520 | CA  | PHE | 240 | 32.913 | -10.422 | 18.870 | 1.00 | 0.00 | 3A4 |
| ATOM | 1521 | CB  | PHE | 240 | 31.825 | -9.669  | 18.040 | 1.00 | 0.00 | 3A4 |
| ATOM | 1522 | CG  | PHE | 240 | 31.881 | -8.134  | 17.899 | 1.00 | 0.00 | 3A4 |
| ATOM | 1523 | CD1 | PHE | 240 | 32.913 | -7.550  | 17.149 | 1.00 | 0.00 | 3A4 |
| ATOM | 1524 | CD2 | PHE | 240 | 31.185 | -7.320  | 18.812 | 1.00 | 0.00 | 3A4 |
| ATOM | 1525 | CE1 | PHE | 240 | 33.312 | -6.223  | 17.382 | 1.00 | 0.00 | 3A4 |
| ATOM | 1526 | CE2 | PHE | 240 | 31.646 | -6.034  | 19.117 | 1.00 | 0.00 | 3A4 |
| ATOM | 1527 | CZ  | PHE | 240 | 32.709 | -5.481  | 18.396 | 1.00 | 0.00 | 3A4 |
| ATOM | 1528 | C   | PHE | 240 | 33.789 | -9.440  | 19.608 | 1.00 | 0.00 | 3A4 |
| ATOM | 1529 | O   | PHE | 240 | 34.906 | -9.202  | 19.168 | 1.00 | 0.00 | 3A4 |
| ATOM | 1530 | N   | PRO | 241 | 33.347 | -8.835  | 20.727 | 1.00 | 0.00 | 3A4 |
| ATOM | 1531 | CA  | PRO | 241 | 34.111 | -7.940  | 21.493 | 1.00 | 0.00 | 3A4 |
| ATOM | 1532 | CD  | PRO | 241 | 32.648 | -9.345  | 21.724 | 1.00 | 0.00 | 3A4 |
| ATOM | 1533 | CB  | PRO | 241 | 33.196 | -7.358  | 22.578 | 1.00 | 0.00 | 3A4 |
| ATOM | 1534 | CG  | PRO | 241 | 32.348 | -8.435  | 22.936 | 1.00 | 0.00 | 3A4 |
| ATOM | 1535 | C   | PRO | 241 | 35.347 | -8.605  | 22.103 | 1.00 | 0.00 | 3A4 |
| ATOM | 1536 | O   | PRO | 241 | 36.396 | -7.992  | 22.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 1537 | N   | ARG | 242 | 35.316 | -9.867  | 22.592 | 1.00 | 0.00 | 3A4 |
| ATOM | 1538 | CA  | ARG | 242 | 36.450 | -10.583 | 23.101 | 1.00 | 0.00 | 3A4 |
| ATOM | 1539 | CB  | ARG | 242 | 35.986 | -11.889 | 23.750 | 1.00 | 0.00 | 3A4 |
| ATOM | 1540 | CG  | ARG | 242 | 35.213 | -11.657 | 25.054 | 1.00 | 0.00 | 3A4 |
| ATOM | 1541 | CD  | ARG | 242 | 34.515 | -12.928 | 25.556 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1542 | NE  | ARG | 242 | 33.717 | -12.581 | 26.784 | 1.00 | 0.00 | 3A4 |
| ATOM | 1543 | CZ  | ARG | 242 | 32.762 | -13.412 | 27.314 | 1.00 | 0.00 | 3A4 |
| ATOM | 1544 | NH1 | ARG | 242 | 32.114 | -13.042 | 28.455 | 1.00 | 0.00 | 3A4 |
| ATOM | 1545 | NH2 | ARG | 242 | 32.444 | -14.603 | 26.725 | 1.00 | 0.00 | 3A4 |
| ATOM | 1546 | C   | ARG | 242 | 37.483 | -10.871 | 22.037 | 1.00 | 0.00 | 3A4 |
| ATOM | 1547 | O   | ARG | 242 | 38.677 | -10.761 | 22.298 | 1.00 | 0.00 | 3A4 |
| ATOM | 1548 | N   | GLU | 243 | 37.044 | -11.158 | 20.784 | 1.00 | 0.00 | 3A4 |
| ATOM | 1549 | CA  | GLU | 243 | 37.911 | -11.394 | 19.638 | 1.00 | 0.00 | 3A4 |
| ATOM | 1550 | CB  | GLU | 243 | 37.126 | -11.846 | 18.383 | 1.00 | 0.00 | 3A4 |
| ATOM | 1551 | CG  | GLU | 243 | 36.626 | -13.298 | 18.452 | 1.00 | 0.00 | 3A4 |
| ATOM | 1552 | CD  | GLU | 243 | 35.759 | -13.581 | 17.219 | 1.00 | 0.00 | 3A4 |
| ATOM | 1553 | OE1 | GLU | 243 | 34.528 | -13.792 | 17.385 | 1.00 | 0.00 | 3A4 |
| ATOM | 1554 | OE2 | GLU | 243 | 36.319 | -13.581 | 16.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 1555 | C   | GLU | 243 | 38.703 | -10.164 | 19.275 | 1.00 | 0.00 | 3A4 |
| ATOM | 1556 | O   | GLU | 243 | 39.908 | -10.244 | 19.057 | 1.00 | 0.00 | 3A4 |
| ATOM | 1557 | N   | VAL | 244 | 38.043 | -8.981  | 19.287 | 1.00 | 0.00 | 3A4 |
| ATOM | 1558 | CA  | VAL | 244 | 38.684 | -7.714  | 18.990 | 1.00 | 0.00 | 3A4 |
| ATOM | 1559 | CB  | VAL | 244 | 37.676 | -6.607  | 18.731 | 1.00 | 0.00 | 3A4 |
| ATOM | 1560 | CG1 | VAL | 244 | 38.391 | -5.314  | 18.259 | 1.00 | 0.00 | 3A4 |
| ATOM | 1561 | CG2 | VAL | 244 | 36.813 | -7.052  | 17.545 | 1.00 | 0.00 | 3A4 |
| ATOM | 1562 | C   | VAL | 244 | 39.649 | -7.327  | 20.084 | 1.00 | 0.00 | 3A4 |
| ATOM | 1563 | O   | VAL | 244 | 40.771 | -6.912  | 19.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 1564 | N   | THR | 245 | 39.257 | -7.535  | 21.357 | 1.00 | 0.00 | 3A4 |
| ATOM | 1565 | CA  | THR | 245 | 40.070 | -7.264  | 22.527 | 1.00 | 0.00 | 3A4 |
| ATOM | 1566 | CB  | THR | 245 | 39.245 | -7.434  | 23.795 | 1.00 | 0.00 | 3A4 |
| ATOM | 1567 | OG1 | THR | 245 | 38.211 | -6.455  | 23.817 | 1.00 | 0.00 | 3A4 |
| ATOM | 1568 | CG2 | THR | 245 | 40.041 | -7.330  | 25.127 | 1.00 | 0.00 | 3A4 |
| ATOM | 1569 | C   | THR | 245 | 41.317 | -8.113  | 22.572 | 1.00 | 0.00 | 3A4 |
| ATOM | 1570 | O   | THR | 245 | 42.397 | -7.605  | 22.842 | 1.00 | 0.00 | 3A4 |
| ATOM | 1571 | N   | ASN | 246 | 41.225 | -9.408  | 22.207 | 1.00 | 0.00 | 3A4 |
| ATOM | 1572 | CA  | ASN | 246 | 42.344 | -10.327 | 22.152 | 1.00 | 0.00 | 3A4 |
| ATOM | 1573 | CB  | ASN | 246 | 41.877 | -11.774 | 21.874 | 1.00 | 0.00 | 3A4 |
| ATOM | 1574 | CG  | ASN | 246 | 41.116 | -12.349 | 23.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 1575 | OD1 | ASN | 246 | 41.128 | -11.808 | 24.187 | 1.00 | 0.00 | 3A4 |
| ATOM | 1576 | ND2 | ASN | 246 | 40.427 | -13.502 | 22.862 | 1.00 | 0.00 | 3A4 |
| ATOM | 1577 | C   | ASN | 246 | 43.340 | -9.950  | 21.088 | 1.00 | 0.00 | 3A4 |
| ATOM | 1578 | O   | ASN | 246 | 44.544 | -10.003 | 21.305 | 1.00 | 0.00 | 3A4 |
| ATOM | 1579 | N   | PHE | 247 | 42.846 | -9.491  | 19.921 | 1.00 | 0.00 | 3A4 |
| ATOM | 1580 | CA  | PHE | 247 | 43.640 | -9.006  | 18.820 | 1.00 | 0.00 | 3A4 |
| ATOM | 1581 | CB  | PHE | 247 | 42.712 | -8.691  | 17.625 | 1.00 | 0.00 | 3A4 |
| ATOM | 1582 | CG  | PHE | 247 | 43.520 | -8.335  | 16.378 | 1.00 | 0.00 | 3A4 |
| ATOM | 1583 | CD1 | PHE | 247 | 44.084 | -9.348  | 15.580 | 1.00 | 0.00 | 3A4 |
| ATOM | 1584 | CD2 | PHE | 247 | 43.817 | -6.990  | 16.065 | 1.00 | 0.00 | 3A4 |
| ATOM | 1585 | CE1 | PHE | 247 | 44.943 | -9.028  | 14.517 | 1.00 | 0.00 | 3A4 |
| ATOM | 1586 | CE2 | PHE | 247 | 44.673 | -6.665  | 15.008 | 1.00 | 0.00 | 3A4 |
| ATOM | 1587 | CZ  | PHE | 247 | 45.245 | -7.686  | 14.243 | 1.00 | 0.00 | 3A4 |
| ATOM | 1588 | C   | PHE | 247 | 44.438 | -7.768  | 19.171 | 1.00 | 0.00 | 3A4 |
| ATOM | 1589 | O   | PHE | 247 | 45.631 | -7.693  | 18.897 | 1.00 | 0.00 | 3A4 |
| ATOM | 1590 | N   | LEU | 248 | 43.781 | -6.766  | 19.795 | 1.00 | 0.00 | 3A4 |
| ATOM | 1591 | CA  | LEU | 248 | 44.374 | -5.480  | 20.131 | 1.00 | 0.00 | 3A4 |
| ATOM | 1592 | CB  | LEU | 248 | 43.291 | -4.473  | 20.599 | 1.00 | 0.00 | 3A4 |
| ATOM | 1593 | CG  | LEU | 248 | 42.423 | -3.985  | 19.422 | 1.00 | 0.00 | 3A4 |
| ATOM | 1594 | CD1 | LEU | 248 | 41.143 | -3.318  | 19.920 | 1.00 | 0.00 | 3A4 |
| ATOM | 1595 | CD2 | LEU | 248 | 43.179 | -3.055  | 18.448 | 1.00 | 0.00 | 3A4 |
| ATOM | 1596 | C   | LEU | 248 | 45.407 | -5.587  | 21.219 | 1.00 | 0.00 | 3A4 |
| ATOM | 1597 | O   | LEU | 248 | 46.458 | -4.959  | 21.175 | 1.00 | 0.00 | 3A4 |
| ATOM | 1598 | N   | ARG | 249 | 45.152 | -6.483  | 22.189 | 1.00 | 0.00 | 3A4 |
| ATOM | 1599 | CA  | ARG | 249 | 46.055 | -6.805  | 23.263 | 1.00 | 0.00 | 3A4 |
| ATOM | 1600 | CB  | ARG | 249 | 45.402 | -7.886  | 24.160 | 1.00 | 0.00 | 3A4 |
| ATOM | 1601 | CG  | ARG | 249 | 44.526 | -7.297  | 25.274 | 1.00 | 0.00 | 3A4 |
| ATOM | 1602 | CD  | ARG | 249 | 45.372 | -6.731  | 26.426 | 1.00 | 0.00 | 3A4 |
| ATOM | 1603 | NE  | ARG | 249 | 44.462 | -6.210  | 27.502 | 1.00 | 0.00 | 3A4 |
| ATOM | 1604 | CZ  | ARG | 249 | 44.932 | -5.795  | 28.722 | 1.00 | 0.00 | 3A4 |
| ATOM | 1605 | NH1 | ARG | 249 | 44.068 | -5.248  | 29.621 | 1.00 | 0.00 | 3A4 |
| ATOM | 1606 | NH2 | ARG | 249 | 46.251 | -5.917  | 29.056 | 1.00 | 0.00 | 3A4 |
| ATOM | 1607 | C   | ARG | 249 | 47.418 | -7.301  | 22.846 | 1.00 | 0.00 | 3A4 |
| ATOM | 1608 | O   | ARG | 249 | 48.444 | -6.897  | 23.385 | 1.00 | 0.00 | 3A4 |
| ATOM | 1609 | N   | LYS | 250 | 47.456 | -8.139  | 21.790 | 1.00 | 0.00 | 3A4 |
| ATOM | 1610 | CA  | LYS | 250 | 48.664 | -8.643  | 21.183 | 1.00 | 0.00 | 3A4 |
| ATOM | 1611 | CB  | LYS | 250 | 48.353 | -9.760  | 20.149 | 1.00 | 0.00 | 3A4 |
| ATOM | 1612 | CG  | LYS | 250 | 47.735 | -11.007 | 20.790 | 1.00 | 0.00 | 3A4 |
| ATOM | 1613 | CD  | LYS | 250 | 47.184 | -11.995 | 19.759 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1614 | CE  | LYS | 250 | 46.472 | -13.190 | 20.404 | 1.00 | 0.00 | 3A4 |
| ATOM | 1615 | NZ  | LYS | 250 | 45.925 | -14.102 | 19.372 | 1.00 | 0.00 | 3A4 |
| ATOM | 1616 | C   | LYS | 250 | 49.481 | -7.572  | 20.506 | 1.00 | 0.00 | 3A4 |
| ATOM | 1617 | O   | LYS | 250 | 50.699 | -7.572  | 20.583 | 1.00 | 0.00 | 3A4 |
| ATOM | 1618 | N   | SER | 251 | 48.809 | -6.584  | 19.881 | 1.00 | 0.00 | 3A4 |
| ATOM | 1619 | CA  | SER | 251 | 49.413 | -5.423  | 19.268 | 1.00 | 0.00 | 3A4 |
| ATOM | 1620 | CB  | SER | 251 | 48.350 | -4.598  | 18.498 | 1.00 | 0.00 | 3A4 |
| ATOM | 1621 | OG  | SER | 251 | 47.705 | -5.410  | 17.524 | 1.00 | 0.00 | 3A4 |
| ATOM | 1622 | C   | SER | 251 | 50.056 | -4.492  | 20.271 | 1.00 | 0.00 | 3A4 |
| ATOM | 1623 | O   | SER | 251 | 51.163 | -4.000  | 20.091 | 1.00 | 0.00 | 3A4 |
| ATOM | 1624 | N   | VAL | 252 | 49.376 | -4.275  | 21.416 | 1.00 | 0.00 | 3A4 |
| ATOM | 1625 | CA  | VAL | 252 | 49.809 | -3.398  | 22.495 | 1.00 | 0.00 | 3A4 |
| ATOM | 1626 | CB  | VAL | 252 | 48.673 | -3.198  | 23.486 | 1.00 | 0.00 | 3A4 |
| ATOM | 1627 | CG1 | VAL | 252 | 49.132 | -2.497  | 24.775 | 1.00 | 0.00 | 3A4 |
| ATOM | 1628 | CG2 | VAL | 252 | 47.610 | -2.462  | 22.625 | 1.00 | 0.00 | 3A4 |
| ATOM | 1629 | C   | VAL | 252 | 51.052 | -3.938  | 23.163 | 1.00 | 0.00 | 3A4 |
| ATOM | 1630 | O   | VAL | 252 | 51.998 | -3.206  | 23.419 | 1.00 | 0.00 | 3A4 |
| ATOM | 1631 | N   | LYS | 253 | 51.108 | -5.271  | 23.380 | 1.00 | 0.00 | 3A4 |
| ATOM | 1632 | CA  | LYS | 253 | 52.243 | -5.976  | 23.944 | 1.00 | 0.00 | 3A4 |
| ATOM | 1633 | CB  | LYS | 253 | 51.887 | -7.462  | 24.155 | 1.00 | 0.00 | 3A4 |
| ATOM | 1634 | CG  | LYS | 253 | 52.903 | -8.297  | 24.953 | 1.00 | 0.00 | 3A4 |
| ATOM | 1635 | CD  | LYS | 253 | 52.410 | -9.721  | 25.224 | 1.00 | 0.00 | 3A4 |
| ATOM | 1636 | CE  | LYS | 253 | 53.418 | -10.563 | 26.018 | 1.00 | 0.00 | 3A4 |
| ATOM | 1637 | NZ  | LYS | 253 | 52.893 | -11.929 | 26.256 | 1.00 | 0.00 | 3A4 |
| ATOM | 1638 | C   | LYS | 253 | 53.481 | -5.877  | 23.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 1639 | O   | LYS | 253 | 54.570 | -5.578  | 23.557 | 1.00 | 0.00 | 3A4 |
| ATOM | 1640 | N   | ARG | 254 | 53.316 | -6.057  | 21.752 | 1.00 | 0.00 | 3A4 |
| ATOM | 1641 | CA  | ARG | 254 | 54.372 | -5.928  | 20.768 | 1.00 | 0.00 | 3A4 |
| ATOM | 1642 | CB  | ARG | 254 | 53.887 | -6.368  | 19.369 | 1.00 | 0.00 | 3A4 |
| ATOM | 1643 | CG  | ARG | 254 | 53.631 | -7.877  | 19.278 | 1.00 | 0.00 | 3A4 |
| ATOM | 1644 | CD  | ARG | 254 | 52.822 | -8.252  | 18.031 | 1.00 | 0.00 | 3A4 |
| ATOM | 1645 | NE  | ARG | 254 | 52.473 | -9.714  | 18.098 | 1.00 | 0.00 | 3A4 |
| ATOM | 1646 | CZ  | ARG | 254 | 51.381 | -10.256 | 17.466 | 1.00 | 0.00 | 3A4 |
| ATOM | 1647 | NH1 | ARG | 254 | 51.133 | -11.591 | 17.596 | 1.00 | 0.00 | 3A4 |
| ATOM | 1648 | NH2 | ARG | 254 | 50.529 | -9.490  | 16.721 | 1.00 | 0.00 | 3A4 |
| ATOM | 1649 | C   | ARG | 254 | 54.899 | -4.517  | 20.676 | 1.00 | 0.00 | 3A4 |
| ATOM | 1650 | O   | ARG | 254 | 56.093 | -4.310  | 20.498 | 1.00 | 0.00 | 3A4 |
| ATOM | 1651 | N   | MET | 255 | 54.021 | -3.508  | 20.844 | 1.00 | 0.00 | 3A4 |
| ATOM | 1652 | CA  | MET | 255 | 54.372 | -2.106  | 20.777 | 1.00 | 0.00 | 3A4 |
| ATOM | 1653 | CB  | MET | 255 | 53.141 | -1.258  | 20.406 | 1.00 | 0.00 | 3A4 |
| ATOM | 1654 | CG  | MET | 255 | 52.816 | -1.403  | 18.917 | 1.00 | 0.00 | 3A4 |
| ATOM | 1655 | SD  | MET | 255 | 51.250 | -0.639  | 18.447 | 1.00 | 0.00 | 3A4 |
| ATOM | 1656 | CE  | MET | 255 | 51.470 | -0.681  | 16.649 | 1.00 | 0.00 | 3A4 |
| ATOM | 1657 | C   | MET | 255 | 55.008 | -1.583  | 22.041 | 1.00 | 0.00 | 3A4 |
| ATOM | 1658 | O   | MET | 255 | 55.687 | -0.563  | 22.027 | 1.00 | 0.00 | 3A4 |
| ATOM | 1659 | N   | LYS | 256 | 54.853 | -2.296  | 23.174 | 1.00 | 0.00 | 3A4 |
| ATOM | 1660 | CA  | LYS | 256 | 55.524 | -1.998  | 24.424 | 1.00 | 0.00 | 3A4 |
| ATOM | 1661 | CB  | LYS | 256 | 54.809 | -2.661  | 25.623 | 1.00 | 0.00 | 3A4 |
| ATOM | 1662 | CG  | LYS | 256 | 53.537 | -1.942  | 26.076 | 1.00 | 0.00 | 3A4 |
| ATOM | 1663 | CD  | LYS | 256 | 52.726 | -2.649  | 27.168 | 1.00 | 0.00 | 3A4 |
| ATOM | 1664 | CE  | LYS | 256 | 53.383 | -2.616  | 28.556 | 1.00 | 0.00 | 3A4 |
| ATOM | 1665 | NZ  | LYS | 256 | 52.487 | -3.206  | 29.579 | 1.00 | 0.00 | 3A4 |
| ATOM | 1666 | C   | LYS | 256 | 56.960 | -2.488  | 24.397 | 1.00 | 0.00 | 3A4 |
| ATOM | 1667 | O   | LYS | 256 | 57.837 | -1.909  | 25.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 1668 | N   | GLU | 257 | 57.220 | -3.565  | 23.619 | 1.00 | 0.00 | 3A4 |
| ATOM | 1669 | CA  | GLU | 257 | 58.527 | -4.164  | 23.444 | 1.00 | 0.00 | 3A4 |
| ATOM | 1670 | CB  | GLU | 257 | 58.421 | -5.661  | 23.058 | 1.00 | 0.00 | 3A4 |
| ATOM | 1671 | CG  | GLU | 257 | 57.813 | -6.520  | 24.182 | 1.00 | 0.00 | 3A4 |
| ATOM | 1672 | CD  | GLU | 257 | 57.607 | -7.953  | 23.679 | 1.00 | 0.00 | 3A4 |
| ATOM | 1673 | OE1 | GLU | 257 | 56.428 | -8.395  | 23.604 | 1.00 | 0.00 | 3A4 |
| ATOM | 1674 | OE2 | GLU | 257 | 58.625 | -8.625  | 23.363 | 1.00 | 0.00 | 3A4 |
| ATOM | 1675 | C   | GLU | 257 | 59.381 | -3.451  | 22.410 | 1.00 | 0.00 | 3A4 |
| ATOM | 1676 | O   | GLU | 257 | 60.407 | -2.870  | 22.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 1677 | N   | SER | 258 | 59.003 | -3.527  | 21.108 | 1.00 | 0.00 | 3A4 |
| ATOM | 1678 | CA  | SER | 258 | 59.766 | -2.938  | 20.026 | 1.00 | 0.00 | 3A4 |
| ATOM | 1679 | CB  | SER | 258 | 61.186 | -3.589  | 19.807 | 1.00 | 0.00 | 3A4 |
| ATOM | 1680 | OG  | SER | 258 | 62.002 | -2.850  | 18.899 | 1.00 | 0.00 | 3A4 |
| ATOM | 1681 | C   | SER | 258 | 58.938 | -3.119  | 18.776 | 1.00 | 0.00 | 3A4 |
| ATOM | 1682 | O   | SER | 258 | 58.503 | -4.225  | 18.459 | 1.00 | 0.00 | 3A4 |
| ATOM | 1683 | N   | ARG | 259 | 58.779 | -2.011  | 18.007 | 1.00 | 0.00 | 3A4 |
| ATOM | 1684 | CA  | ARG | 259 | 58.391 | -2.013  | 16.612 | 1.00 | 0.00 | 3A4 |
| ATOM | 1685 | CB  | ARG | 259 | 56.880 | -1.758  | 16.329 | 1.00 | 0.00 | 3A4 |



|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 1686 | CG  | ARG | 259 | 55.968 | -2.939 | 16.688 | 1.00 | 0.00 | 3A4 |
| ATOM | 1687 | CD  | ARG | 259 | 54.607 | -2.858 | 15.987 | 1.00 | 0.00 | 3A4 |
| ATOM | 1688 | NE  | ARG | 259 | 53.744 | -4.000 | 16.458 | 1.00 | 0.00 | 3A4 |
| ATOM | 1689 | CZ  | ARG | 259 | 52.617 | -4.411 | 15.791 | 1.00 | 0.00 | 3A4 |
| ATOM | 1690 | NH1 | ARG | 259 | 51.837 | -5.390 | 16.332 | 1.00 | 0.00 | 3A4 |
| ATOM | 1691 | NH2 | ARG | 259 | 52.247 | -3.859 | 14.598 | 1.00 | 0.00 | 3A4 |
| ATOM | 1692 | C   | ARG | 259 | 59.262 | -0.943 | 16.000 | 1.00 | 0.00 | 3A4 |
| ATOM | 1693 | O   | ARG | 259 | 60.401 | -1.220 | 15.626 | 1.00 | 0.00 | 3A4 |
| ATOM | 1694 | N   | LEU | 260 | 58.752 | 0.314  | 15.898 | 1.00 | 0.00 | 3A4 |
| ATOM | 1695 | CA  | LEU | 260 | 59.502 | 1.436  | 15.373 | 1.00 | 0.00 | 3A4 |
| ATOM | 1696 | CB  | LEU | 260 | 59.602 | 1.425  | 13.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 1697 | CG  | LEU | 260 | 60.595 | 2.428  | 13.175 | 1.00 | 0.00 | 3A4 |
| ATOM | 1698 | CD1 | LEU | 260 | 62.054 | 2.163  | 13.599 | 1.00 | 0.00 | 3A4 |
| ATOM | 1699 | CD2 | LEU | 260 | 60.467 | 2.427  | 11.640 | 1.00 | 0.00 | 3A4 |
| ATOM | 1700 | C   | LEU | 260 | 58.790 | 2.670  | 15.874 | 1.00 | 0.00 | 3A4 |
| ATOM | 1701 | O   | LEU | 260 | 58.005 | 3.291  | 15.159 | 1.00 | 0.00 | 3A4 |
| ATOM | 1702 | N   | GLU | 261 | 59.062 | 3.038  | 17.155 | 1.00 | 0.00 | 3A4 |
| ATOM | 1703 | CA  | GLU | 261 | 58.441 | 4.130  | 17.884 | 1.00 | 0.00 | 3A4 |
| ATOM | 1704 | CB  | GLU | 261 | 57.742 | 3.683  | 19.213 | 1.00 | 0.00 | 3A4 |
| ATOM | 1705 | CG  | GLU | 261 | 58.554 | 2.841  | 20.229 | 1.00 | 0.00 | 3A4 |
| ATOM | 1706 | CD  | GLU | 261 | 58.717 | 1.386  | 19.761 | 1.00 | 0.00 | 3A4 |
| ATOM | 1707 | OE1 | GLU | 261 | 59.884 | 0.942  | 19.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 1708 | OE2 | GLU | 261 | 57.675 | 0.701  | 19.572 | 1.00 | 0.00 | 3A4 |
| ATOM | 1709 | C   | GLU | 261 | 59.482 | 5.186  | 18.166 | 1.00 | 0.00 | 3A4 |
| ATOM | 1710 | O   | GLU | 261 | 60.619 | 4.877  | 18.523 | 1.00 | 0.00 | 3A4 |
| ATOM | 1711 | N   | ASP | 262 | 59.067 | 6.478  | 17.991 | 1.00 | 0.00 | 3A4 |
| ATOM | 1712 | CA  | ASP | 262 | 59.771 | 7.738  | 18.239 | 1.00 | 0.00 | 3A4 |
| ATOM | 1713 | CB  | ASP | 262 | 60.392 | 7.859  | 19.674 | 1.00 | 0.00 | 3A4 |
| ATOM | 1714 | CG  | ASP | 262 | 59.293 | 7.671  | 20.735 | 1.00 | 0.00 | 3A4 |
| ATOM | 1715 | OD1 | ASP | 262 | 59.392 | 6.700  | 21.533 | 1.00 | 0.00 | 3A4 |
| ATOM | 1716 | OD2 | ASP | 262 | 58.341 | 8.497  | 20.759 | 1.00 | 0.00 | 3A4 |
| ATOM | 1717 | C   | ASP | 262 | 60.828 | 8.011  | 17.175 | 1.00 | 0.00 | 3A4 |
| ATOM | 1718 | O   | ASP | 262 | 62.015 | 8.125  | 17.477 | 1.00 | 0.00 | 3A4 |
| ATOM | 1719 | N   | THR | 263 | 60.385 | 8.087  | 15.889 | 1.00 | 0.00 | 3A4 |
| ATOM | 1720 | CA  | THR | 263 | 61.231 | 8.151  | 14.709 | 1.00 | 0.00 | 3A4 |
| ATOM | 1721 | CB  | THR | 263 | 61.257 | 6.828  | 13.922 | 1.00 | 0.00 | 3A4 |
| ATOM | 1722 | OG1 | THR | 263 | 59.962 | 6.247  | 13.768 | 1.00 | 0.00 | 3A4 |
| ATOM | 1723 | CG2 | THR | 263 | 62.163 | 5.831  | 14.677 | 1.00 | 0.00 | 3A4 |
| ATOM | 1724 | C   | THR | 263 | 60.819 | 9.346  | 13.857 | 1.00 | 0.00 | 3A4 |
| ATOM | 1725 | O   | THR | 263 | 61.248 | 10.466 | 14.127 | 1.00 | 0.00 | 3A4 |
| ATOM | 1726 | N   | GLN | 264 | 60.017 | 9.120  | 12.773 | 1.00 | 0.00 | 3A4 |
| ATOM | 1727 | CA  | GLN | 264 | 59.831 | 10.032 | 11.649 | 1.00 | 0.00 | 3A4 |
| ATOM | 1728 | CB  | GLN | 264 | 59.812 | 9.263  | 10.288 | 1.00 | 0.00 | 3A4 |
| ATOM | 1729 | CG  | GLN | 264 | 61.018 | 8.324  | 10.094 | 1.00 | 0.00 | 3A4 |
| ATOM | 1730 | CD  | GLN | 264 | 60.951 | 7.671  | 8.710  | 1.00 | 0.00 | 3A4 |
| ATOM | 1731 | OE1 | GLN | 264 | 61.775 | 7.968  | 7.846  | 1.00 | 0.00 | 3A4 |
| ATOM | 1732 | NE2 | GLN | 264 | 59.961 | 6.763  | 8.489  | 1.00 | 0.00 | 3A4 |
| ATOM | 1733 | C   | GLN | 264 | 58.564 | 10.861 | 11.768 | 1.00 | 0.00 | 3A4 |
| ATOM | 1734 | O   | GLN | 264 | 57.907 | 10.891 | 12.808 | 1.00 | 0.00 | 3A4 |
| ATOM | 1735 | N   | LYS | 265 | 58.214 | 11.556 | 10.645 | 1.00 | 0.00 | 3A4 |
| ATOM | 1736 | CA  | LYS | 265 | 57.091 | 12.459 | 10.453 | 1.00 | 0.00 | 3A4 |
| ATOM | 1737 | CB  | LYS | 265 | 57.471 | 13.608 | 9.470  | 1.00 | 0.00 | 3A4 |
| ATOM | 1738 | CG  | LYS | 265 | 56.414 | 14.703 | 9.209  | 1.00 | 0.00 | 3A4 |
| ATOM | 1739 | CD  | LYS | 265 | 55.986 | 15.485 | 10.458 | 1.00 | 0.00 | 3A4 |
| ATOM | 1740 | CE  | LYS | 265 | 55.004 | 16.618 | 10.140 | 1.00 | 0.00 | 3A4 |
| ATOM | 1741 | NZ  | LYS | 265 | 54.585 | 17.323 | 11.374 | 1.00 | 0.00 | 3A4 |
| ATOM | 1742 | C   | LYS | 265 | 55.895 | 11.698 | 9.920  | 1.00 | 0.00 | 3A4 |
| ATOM | 1743 | O   | LYS | 265 | 54.757 | 11.957 | 10.308 | 1.00 | 0.00 | 3A4 |
| ATOM | 1744 | N   | HIS | 266 | 56.161 | 10.712 | 9.017  | 1.00 | 0.00 | 3A4 |
| ATOM | 1745 | CA  | HIS | 266 | 55.192 | 9.789  | 8.453  | 1.00 | 0.00 | 3A4 |
| ATOM | 1746 | ND1 | HIS | 266 | 53.213 | 11.484 | 6.555  | 1.00 | 0.00 | 3A4 |
| ATOM | 1747 | CG  | HIS | 266 | 54.551 | 11.168 | 6.457  | 1.00 | 0.00 | 3A4 |
| ATOM | 1748 | CB  | HIS | 266 | 55.138 | 9.857  | 6.906  | 1.00 | 0.00 | 3A4 |
| ATOM | 1749 | NE2 | HIS | 266 | 54.234 | 13.294 | 5.769  | 1.00 | 0.00 | 3A4 |
| ATOM | 1750 | CD2 | HIS | 266 | 55.161 | 12.287 | 5.977  | 1.00 | 0.00 | 3A4 |
| ATOM | 1751 | CE1 | HIS | 266 | 53.080 | 12.764 | 6.128  | 1.00 | 0.00 | 3A4 |
| ATOM | 1752 | C   | HIS | 266 | 55.520 | 8.402  | 8.961  | 1.00 | 0.00 | 3A4 |
| ATOM | 1753 | O   | HIS | 266 | 55.595 | 7.432  | 8.208  | 1.00 | 0.00 | 3A4 |
| ATOM | 1754 | N   | ARG | 267 | 55.681 | 8.319  | 10.306 | 1.00 | 0.00 | 3A4 |
| ATOM | 1755 | CA  | ARG | 267 | 55.787 | 7.112  | 11.088 | 1.00 | 0.00 | 3A4 |
| ATOM | 1756 | CB  | ARG | 267 | 57.206 | 6.450  | 11.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 1757 | CG  | ARG | 267 | 57.342 | 5.024  | 11.602 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 1758 | CD  | ARG | 267 | 56.433 | 3.983  | 10.915 | 1.00 | 0.00 | 3A4 |
| ATOM | 1759 | NE  | ARG | 267 | 56.515 | 2.666  | 11.644 | 1.00 | 0.00 | 3A4 |
| ATOM | 1760 | CZ  | ARG | 267 | 55.718 | 2.342  | 12.715 | 1.00 | 0.00 | 3A4 |
| ATOM | 1761 | NH1 | ARG | 267 | 55.829 | 1.104  | 13.280 | 1.00 | 0.00 | 3A4 |
| ATOM | 1762 | NH2 | ARG | 267 | 54.819 | 3.229  | 13.235 | 1.00 | 0.00 | 3A4 |
| ATOM | 1763 | C   | ARG | 267 | 55.443 | 7.575  | 12.488 | 1.00 | 0.00 | 3A4 |
| ATOM | 1764 | O   | ARG | 267 | 55.403 | 8.776  | 12.757 | 1.00 | 0.00 | 3A4 |
| ATOM | 1765 | N   | VAL | 268 | 55.180 | 6.600  | 13.409 | 1.00 | 0.00 | 3A4 |
| ATOM | 1766 | CA  | VAL | 268 | 54.850 | 6.700  | 14.830 | 1.00 | 0.00 | 3A4 |
| ATOM | 1767 | CB  | VAL | 268 | 55.608 | 7.738  | 15.672 | 1.00 | 0.00 | 3A4 |
| ATOM | 1768 | CG1 | VAL | 268 | 55.286 | 7.564  | 17.181 | 1.00 | 0.00 | 3A4 |
| ATOM | 1769 | CG2 | VAL | 268 | 57.124 | 7.555  | 15.459 | 1.00 | 0.00 | 3A4 |
| ATOM | 1770 | C   | VAL | 268 | 53.347 | 6.859  | 14.949 | 1.00 | 0.00 | 3A4 |
| ATOM | 1771 | O   | VAL | 268 | 52.814 | 7.966  | 14.876 | 1.00 | 0.00 | 3A4 |
| ATOM | 1772 | N   | ASP | 269 | 52.650 | 5.703  | 15.128 | 1.00 | 0.00 | 3A4 |
| ATOM | 1773 | CA  | ASP | 269 | 51.217 | 5.484  | 15.039 | 1.00 | 0.00 | 3A4 |
| ATOM | 1774 | CB  | ASP | 269 | 50.952 | 4.008  | 14.629 | 1.00 | 0.00 | 3A4 |
| ATOM | 1775 | CG  | ASP | 269 | 51.584 | 2.963  | 15.562 | 1.00 | 0.00 | 3A4 |
| ATOM | 1776 | OD1 | ASP | 269 | 52.585 | 2.329  | 15.136 | 1.00 | 0.00 | 3A4 |
| ATOM | 1777 | OD2 | ASP | 269 | 51.040 | 2.734  | 16.671 | 1.00 | 0.00 | 3A4 |
| ATOM | 1778 | C   | ASP | 269 | 50.513 | 5.855  | 16.322 | 1.00 | 0.00 | 3A4 |
| ATOM | 1779 | O   | ASP | 269 | 51.163 | 6.144  | 17.324 | 1.00 | 0.00 | 3A4 |
| ATOM | 1780 | N   | PHE | 270 | 49.161 | 5.834  | 16.331 | 1.00 | 0.00 | 3A4 |
| ATOM | 1781 | CA  | PHE | 270 | 48.362 | 6.204  | 17.490 | 1.00 | 0.00 | 3A4 |
| ATOM | 1782 | CB  | PHE | 270 | 46.855 | 6.258  | 17.148 | 1.00 | 0.00 | 3A4 |
| ATOM | 1783 | CG  | PHE | 270 | 45.990 | 6.766  | 18.282 | 1.00 | 0.00 | 3A4 |
| ATOM | 1784 | CD1 | PHE | 270 | 45.280 | 5.854  | 19.081 | 1.00 | 0.00 | 3A4 |
| ATOM | 1785 | CD2 | PHE | 270 | 46.020 | 8.114  | 18.661 | 1.00 | 0.00 | 3A4 |
| ATOM | 1786 | CE1 | PHE | 270 | 44.531 | 6.282  | 20.177 | 1.00 | 0.00 | 3A4 |
| ATOM | 1787 | CE2 | PHE | 270 | 45.309 | 8.546  | 19.789 | 1.00 | 0.00 | 3A4 |
| ATOM | 1788 | CZ  | PHE | 270 | 44.542 | 7.634  | 20.522 | 1.00 | 0.00 | 3A4 |
| ATOM | 1789 | C   | PHE | 270 | 48.565 | 5.305  | 18.696 | 1.00 | 0.00 | 3A4 |
| ATOM | 1790 | O   | PHE | 270 | 48.623 | 5.789  | 19.822 | 1.00 | 0.00 | 3A4 |
| ATOM | 1791 | N   | LEU | 271 | 48.707 | 3.980  | 18.488 | 1.00 | 0.00 | 3A4 |
| ATOM | 1792 | CA  | LEU | 271 | 48.911 | 3.039  | 19.569 | 1.00 | 0.00 | 3A4 |
| ATOM | 1793 | CB  | LEU | 271 | 48.798 | 1.584  | 19.058 | 1.00 | 0.00 | 3A4 |
| ATOM | 1794 | CG  | LEU | 271 | 47.377 | 1.034  | 18.852 | 1.00 | 0.00 | 3A4 |
| ATOM | 1795 | CD1 | LEU | 271 | 47.422 | -0.399 | 18.277 | 1.00 | 0.00 | 3A4 |
| ATOM | 1796 | CD2 | LEU | 271 | 46.550 | 1.035  | 20.150 | 1.00 | 0.00 | 3A4 |
| ATOM | 1797 | C   | LEU | 271 | 50.247 | 3.247  | 20.287 | 1.00 | 0.00 | 3A4 |
| ATOM | 1798 | O   | LEU | 271 | 50.309 | 3.283  | 21.510 | 1.00 | 0.00 | 3A4 |
| ATOM | 1799 | N   | GLN | 272 | 51.325 | 3.513  | 19.518 | 1.00 | 0.00 | 3A4 |
| ATOM | 1800 | CA  | GLN | 272 | 52.641 | 3.856  | 20.018 | 1.00 | 0.00 | 3A4 |
| ATOM | 1801 | CB  | GLN | 272 | 53.651 | 3.973  | 18.871 | 1.00 | 0.00 | 3A4 |
| ATOM | 1802 | CG  | GLN | 272 | 53.989 | 2.568  | 18.334 | 1.00 | 0.00 | 3A4 |
| ATOM | 1803 | CD  | GLN | 272 | 54.908 | 2.656  | 17.119 | 1.00 | 0.00 | 3A4 |
| ATOM | 1804 | OE1 | GLN | 272 | 55.225 | 3.735  | 16.626 | 1.00 | 0.00 | 3A4 |
| ATOM | 1805 | NE2 | GLN | 272 | 55.347 | 1.475  | 16.611 | 1.00 | 0.00 | 3A4 |
| ATOM | 1806 | C   | GLN | 272 | 52.646 | 5.136  | 20.813 | 1.00 | 0.00 | 3A4 |
| ATOM | 1807 | O   | GLN | 272 | 53.254 | 5.214  | 21.874 | 1.00 | 0.00 | 3A4 |
| ATOM | 1808 | N   | LEU | 273 | 51.883 | 6.155  | 20.356 | 1.00 | 0.00 | 3A4 |
| ATOM | 1809 | CA  | LEU | 273 | 51.695 | 7.415  | 21.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 1810 | CB  | LEU | 273 | 50.926 | 8.433  | 20.166 | 1.00 | 0.00 | 3A4 |
| ATOM | 1811 | CG  | LEU | 273 | 51.785 | 8.888  | 18.948 | 1.00 | 0.00 | 3A4 |
| ATOM | 1812 | CD1 | LEU | 273 | 50.959 | 9.439  | 17.771 | 1.00 | 0.00 | 3A4 |
| ATOM | 1813 | CD2 | LEU | 273 | 52.899 | 9.882  | 19.332 | 1.00 | 0.00 | 3A4 |
| ATOM | 1814 | C   | LEU | 273 | 50.983 | 7.274  | 22.346 | 1.00 | 0.00 | 3A4 |
| ATOM | 1815 | O   | LEU | 273 | 51.365 | 7.895  | 23.329 | 1.00 | 0.00 | 3A4 |
| ATOM | 1816 | N   | MET | 274 | 49.964 | 6.395  | 22.412 | 1.00 | 0.00 | 3A4 |
| ATOM | 1817 | CA  | MET | 274 | 49.244 | 6.073  | 23.621 | 1.00 | 0.00 | 3A4 |
| ATOM | 1818 | CB  | MET | 274 | 47.977 | 5.254  | 23.316 | 1.00 | 0.00 | 3A4 |
| ATOM | 1819 | CG  | MET | 274 | 46.828 | 6.090  | 22.751 | 1.00 | 0.00 | 3A4 |
| ATOM | 1820 | SD  | MET | 274 | 45.317 | 6.067  | 23.770 | 1.00 | 0.00 | 3A4 |
| ATOM | 1821 | CE  | MET | 274 | 45.991 | 6.940  | 25.218 | 1.00 | 0.00 | 3A4 |
| ATOM | 1822 | C   | MET | 274 | 50.109 | 5.325  | 24.619 | 1.00 | 0.00 | 3A4 |
| ATOM | 1823 | O   | MET | 274 | 50.038 | 5.567  | 25.819 | 1.00 | 0.00 | 3A4 |
| ATOM | 1824 | N   | ILE | 275 | 50.988 | 4.417  | 24.131 | 1.00 | 0.00 | 3A4 |
| ATOM | 1825 | CA  | ILE | 275 | 51.851 | 3.564  | 24.931 | 1.00 | 0.00 | 3A4 |
| ATOM | 1826 | CB  | ILE | 275 | 52.467 | 2.441  | 24.078 | 1.00 | 0.00 | 3A4 |
| ATOM | 1827 | CG2 | ILE | 275 | 53.965 | 2.545  | 23.648 | 1.00 | 0.00 | 3A4 |
| ATOM | 1828 | CG1 | ILE | 275 | 52.209 | 1.038  | 24.643 | 1.00 | 0.00 | 3A4 |
| ATOM | 1829 | CD  | ILE | 275 | 51.787 | 0.081  | 23.536 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 1830 | C   | ILE | 275 | 52.925 | 4.329  | 25.660 | 1.00 | 0.00 | 3A4 |
| ATOM | 1831 | O   | ILE | 275 | 53.323 | 3.975  | 26.764 | 1.00 | 0.00 | 3A4 |
| ATOM | 1832 | N   | ASP | 276 | 53.392 | 5.425  | 25.033 | 1.00 | 0.00 | 3A4 |
| ATOM | 1833 | CA  | ASP | 276 | 54.488 | 6.233  | 25.491 | 1.00 | 0.00 | 3A4 |
| ATOM | 1834 | CB  | ASP | 276 | 55.375 | 6.635  | 24.263 | 1.00 | 0.00 | 3A4 |
| ATOM | 1835 | CG  | ASP | 276 | 56.766 | 7.177  | 24.648 | 1.00 | 0.00 | 3A4 |
| ATOM | 1836 | OD1 | ASP | 276 | 57.527 | 6.432  | 25.323 | 1.00 | 0.00 | 3A4 |
| ATOM | 1837 | OD2 | ASP | 276 | 57.080 | 8.336  | 24.266 | 1.00 | 0.00 | 3A4 |
| ATOM | 1838 | C   | ASP | 276 | 53.994 | 7.467  | 26.229 | 1.00 | 0.00 | 3A4 |
| ATOM | 1839 | O   | ASP | 276 | 54.738 | 8.023  | 27.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 1840 | N   | SER | 277 | 52.734 | 7.918  | 25.959 | 1.00 | 0.00 | 3A4 |
| ATOM | 1841 | CA  | SER | 277 | 51.962 | 9.005  | 26.574 | 1.00 | 0.00 | 3A4 |
| ATOM | 1842 | CB  | SER | 277 | 51.494 | 8.689  | 28.034 | 1.00 | 0.00 | 3A4 |
| ATOM | 1843 | OG  | SER | 277 | 52.536 | 8.498  | 28.989 | 1.00 | 0.00 | 3A4 |
| ATOM | 1844 | C   | SER | 277 | 52.586 | 10.401 | 26.477 | 1.00 | 0.00 | 3A4 |
| ATOM | 1845 | O   | SER | 277 | 53.547 | 10.719 | 27.177 | 1.00 | 0.00 | 3A4 |
| ATOM | 1846 | N   | GLN | 278 | 52.027 | 11.259 | 25.584 | 1.00 | 0.00 | 3A4 |
| ATOM | 1847 | CA  | GLN | 278 | 52.576 | 12.557 | 25.230 | 1.00 | 0.00 | 3A4 |
| ATOM | 1848 | CB  | GLN | 278 | 53.079 | 12.585 | 23.748 | 1.00 | 0.00 | 3A4 |
| ATOM | 1849 | CG  | GLN | 278 | 52.289 | 11.752 | 22.708 | 1.00 | 0.00 | 3A4 |
| ATOM | 1850 | CD  | GLN | 278 | 50.896 | 12.317 | 22.436 | 1.00 | 0.00 | 3A4 |
| ATOM | 1851 | OE1 | GLN | 278 | 49.896 | 11.703 | 22.807 | 1.00 | 0.00 | 3A4 |
| ATOM | 1852 | NE2 | GLN | 278 | 50.821 | 13.500 | 21.767 | 1.00 | 0.00 | 3A4 |
| ATOM | 1853 | C   | GLN | 278 | 51.568 | 13.647 | 25.534 | 1.00 | 0.00 | 3A4 |
| ATOM | 1854 | O   | GLN | 278 | 51.306 | 14.524 | 24.712 | 1.00 | 0.00 | 3A4 |
| ATOM | 1855 | N   | ASN | 279 | 51.016 | 13.632 | 26.775 | 1.00 | 0.00 | 3A4 |
| ATOM | 1856 | CA  | ASN | 279 | 50.193 | 14.697 | 27.310 | 1.00 | 0.00 | 3A4 |
| ATOM | 1857 | CB  | ASN | 279 | 48.716 | 14.690 | 26.781 | 1.00 | 0.00 | 3A4 |
| ATOM | 1858 | CG  | ASN | 279 | 47.973 | 15.999 | 27.107 | 1.00 | 0.00 | 3A4 |
| ATOM | 1859 | OD1 | ASN | 279 | 47.305 | 16.089 | 28.136 | 1.00 | 0.00 | 3A4 |
| ATOM | 1860 | ND2 | ASN | 279 | 48.086 | 17.026 | 26.221 | 1.00 | 0.00 | 3A4 |
| ATOM | 1861 | C   | ASN | 279 | 50.239 | 14.505 | 28.808 | 1.00 | 0.00 | 3A4 |
| ATOM | 1862 | O   | ASN | 279 | 50.626 | 15.409 | 29.546 | 1.00 | 0.00 | 3A4 |
| ATOM | 1863 | N   | SER | 280 | 49.821 | 13.295 | 29.277 | 1.00 | 0.00 | 3A4 |
| ATOM | 1864 | CA  | SER | 280 | 49.736 | 12.901 | 30.674 | 1.00 | 0.00 | 3A4 |
| ATOM | 1865 | CB  | SER | 280 | 48.334 | 12.330 | 31.056 | 1.00 | 0.00 | 3A4 |
| ATOM | 1866 | OG  | SER | 280 | 47.313 | 13.268 | 30.740 | 1.00 | 0.00 | 3A4 |
| ATOM | 1867 | C   | SER | 280 | 50.810 | 11.870 | 30.942 | 1.00 | 0.00 | 3A4 |
| ATOM | 1868 | O   | SER | 280 | 51.635 | 11.569 | 30.079 | 1.00 | 0.00 | 3A4 |
| ATOM | 1869 | N   | LYS | 281 | 50.813 | 11.317 | 32.183 | 1.00 | 0.00 | 3A4 |
| ATOM | 1870 | CA  | LYS | 281 | 51.810 | 10.412 | 32.724 | 1.00 | 0.00 | 3A4 |
| ATOM | 1871 | CB  | LYS | 281 | 52.318 | 10.863 | 34.135 | 1.00 | 0.00 | 3A4 |
| ATOM | 1872 | CG  | LYS | 281 | 51.368 | 10.740 | 35.357 | 1.00 | 0.00 | 3A4 |
| ATOM | 1873 | CD  | LYS | 281 | 50.099 | 11.612 | 35.328 | 1.00 | 0.00 | 3A4 |
| ATOM | 1874 | CE  | LYS | 281 | 49.241 | 11.508 | 36.598 | 1.00 | 0.00 | 3A4 |
| ATOM | 1875 | NZ  | LYS | 281 | 48.695 | 10.139 | 36.770 | 1.00 | 0.00 | 3A4 |
| ATOM | 1876 | C   | LYS | 281 | 51.259 | 9.009  | 32.800 | 1.00 | 0.00 | 3A4 |
| ATOM | 1877 | O   | LYS | 281 | 50.051 | 8.792  | 32.725 | 1.00 | 0.00 | 3A4 |
| ATOM | 1878 | N   | GLU | 282 | 52.179 | 8.025  | 33.003 | 1.00 | 0.00 | 3A4 |
| ATOM | 1879 | CA  | GLU | 282 | 51.902 | 6.623  | 33.252 | 1.00 | 0.00 | 3A4 |
| ATOM | 1880 | CB  | GLU | 282 | 52.839 | 5.684  | 32.439 | 1.00 | 0.00 | 3A4 |
| ATOM | 1881 | CG  | GLU | 282 | 54.355 | 5.905  | 32.633 | 1.00 | 0.00 | 3A4 |
| ATOM | 1882 | CD  | GLU | 282 | 55.125 | 5.055  | 31.617 | 1.00 | 0.00 | 3A4 |
| ATOM | 1883 | OE1 | GLU | 282 | 54.983 | 5.322  | 30.393 | 1.00 | 0.00 | 3A4 |
| ATOM | 1884 | OE2 | GLU | 282 | 55.866 | 4.133  | 32.049 | 1.00 | 0.00 | 3A4 |
| ATOM | 1885 | C   | GLU | 282 | 52.026 | 6.378  | 34.739 | 1.00 | 0.00 | 3A4 |
| ATOM | 1886 | O   | GLU | 282 | 52.842 | 7.002  | 35.416 | 1.00 | 0.00 | 3A4 |
| ATOM | 1887 | N   | THR | 283 | 51.169 | 5.468  | 35.281 | 1.00 | 0.00 | 3A4 |
| ATOM | 1888 | CA  | THR | 283 | 50.949 | 5.262  | 36.708 | 1.00 | 0.00 | 3A4 |
| ATOM | 1889 | CB  | THR | 283 | 49.462 | 5.076  | 37.037 | 1.00 | 0.00 | 3A4 |
| ATOM | 1890 | OG1 | THR | 283 | 48.843 | 4.071  | 36.236 | 1.00 | 0.00 | 3A4 |
| ATOM | 1891 | CG2 | THR | 283 | 48.746 | 6.425  | 36.797 | 1.00 | 0.00 | 3A4 |
| ATOM | 1892 | C   | THR | 283 | 51.786 | 4.117  | 37.266 | 1.00 | 0.00 | 3A4 |
| ATOM | 1893 | O   | THR | 283 | 51.843 | 3.935  | 38.481 | 1.00 | 0.00 | 3A4 |
| ATOM | 1894 | N   | GLU | 284 | 52.457 | 3.329  | 36.385 | 1.00 | 0.00 | 3A4 |
| ATOM | 1895 | CA  | GLU | 284 | 53.336 | 2.253  | 36.792 | 1.00 | 0.00 | 3A4 |
| ATOM | 1896 | CB  | GLU | 284 | 52.583 | 0.907  | 37.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 1897 | CG  | GLU | 284 | 53.427 | -0.211 | 37.670 | 1.00 | 0.00 | 3A4 |
| ATOM | 1898 | CD  | GLU | 284 | 52.553 | -1.452 | 37.873 | 1.00 | 0.00 | 3A4 |
| ATOM | 1899 | OE1 | GLU | 284 | 52.075 | -2.014 | 36.851 | 1.00 | 0.00 | 3A4 |
| ATOM | 1900 | OE2 | GLU | 284 | 52.352 | -1.855 | 39.051 | 1.00 | 0.00 | 3A4 |
| ATOM | 1901 | C   | GLU | 284 | 54.393 | 2.152  | 35.719 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 1902 | O   | GLU | 284 | 55.397 | 2.861  | 35.770 | 1.00 | 0.00 | 3A4 |
| ATOM | 1903 | N   | SER | 285 | 54.186 | 1.256  | 34.721 | 1.00 | 0.00 | 3A4 |
| ATOM | 1904 | CA  | SER | 285 | 55.139 | 0.973  | 33.669 | 1.00 | 0.00 | 3A4 |
| ATOM | 1905 | CB  | SER | 285 | 56.281 | -0.008 | 34.108 | 1.00 | 0.00 | 3A4 |
| ATOM | 1906 | OG  | SER | 285 | 55.800 | -1.171 | 34.781 | 1.00 | 0.00 | 3A4 |
| ATOM | 1907 | C   | SER | 285 | 54.331 | 0.438  | 32.510 | 1.00 | 0.00 | 3A4 |
| ATOM | 1908 | O   | SER | 285 | 54.522 | -0.694 | 32.066 | 1.00 | 0.00 | 3A4 |
| ATOM | 1909 | N   | HIS | 286 | 53.396 | 1.275  | 31.998 | 1.00 | 0.00 | 3A4 |
| ATOM | 1910 | CA  | HIS | 286 | 52.522 | 0.926  | 30.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 1911 | ND1 | HIS | 286 | 49.824 | 1.672  | 32.816 | 1.00 | 0.00 | 3A4 |
| ATOM | 1912 | CG  | HIS | 286 | 50.594 | 0.542  | 32.645 | 1.00 | 0.00 | 3A4 |
| ATOM | 1913 | CB  | HIS | 286 | 51.264 | 0.113  | 31.356 | 1.00 | 0.00 | 3A4 |
| ATOM | 1914 | NE2 | HIS | 286 | 49.782 | 0.592  | 34.753 | 1.00 | 0.00 | 3A4 |
| ATOM | 1915 | CD2 | HIS | 286 | 50.557 | -0.106 | 33.843 | 1.00 | 0.00 | 3A4 |
| ATOM | 1916 | CE1 | HIS | 286 | 49.366 | 1.652  | 34.090 | 1.00 | 0.00 | 3A4 |
| ATOM | 1917 | C   | HIS | 286 | 52.192 | 2.222  | 30.200 | 1.00 | 0.00 | 3A4 |
| ATOM | 1918 | O   | HIS | 286 | 53.089 | 2.937  | 29.758 | 1.00 | 0.00 | 3A4 |
| ATOM | 1919 | N   | LYS | 287 | 50.878 | 2.537  | 30.069 | 1.00 | 0.00 | 3A4 |
| ATOM | 1920 | CA  | LYS | 287 | 50.317 | 3.652  | 29.338 | 1.00 | 0.00 | 3A4 |
| ATOM | 1921 | CB  | LYS | 287 | 49.136 | 3.180  | 28.453 | 1.00 | 0.00 | 3A4 |
| ATOM | 1922 | CG  | LYS | 287 | 49.553 | 2.209  | 27.349 | 1.00 | 0.00 | 3A4 |
| ATOM | 1923 | CD  | LYS | 287 | 48.717 | 2.529  | 26.095 | 1.00 | 0.00 | 3A4 |
| ATOM | 1924 | CE  | LYS | 287 | 48.931 | 1.795  | 24.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 1925 | NZ  | LYS | 287 | 47.885 | 2.079  | 23.732 | 1.00 | 0.00 | 3A4 |
| ATOM | 1926 | C   | LYS | 287 | 49.794 | 4.698  | 30.287 | 1.00 | 0.00 | 3A4 |
| ATOM | 1927 | O   | LYS | 287 | 49.872 | 4.548  | 31.504 | 1.00 | 0.00 | 3A4 |
| ATOM | 1928 | N   | ALA | 288 | 49.185 | 5.771  | 29.701 | 1.00 | 0.00 | 3A4 |
| ATOM | 1929 | CA  | ALA | 288 | 48.374 | 6.783  | 30.350 | 1.00 | 0.00 | 3A4 |
| ATOM | 1930 | CB  | ALA | 288 | 48.615 | 8.202  | 29.810 | 1.00 | 0.00 | 3A4 |
| ATOM | 1931 | C   | ALA | 288 | 46.906 | 6.403  | 30.192 | 1.00 | 0.00 | 3A4 |
| ATOM | 1932 | O   | ALA | 288 | 46.333 | 6.618  | 29.125 | 1.00 | 0.00 | 3A4 |
| ATOM | 1933 | N   | LEU | 289 | 46.245 | 5.810  | 31.226 | 1.00 | 0.00 | 3A4 |
| ATOM | 1934 | CA  | LEU | 289 | 46.774 | 5.489  | 32.535 | 1.00 | 0.00 | 3A4 |
| ATOM | 1935 | CB  | LEU | 289 | 46.349 | 6.484  | 33.668 | 1.00 | 0.00 | 3A4 |
| ATOM | 1936 | CG  | LEU | 289 | 44.839 | 6.740  | 33.920 | 1.00 | 0.00 | 3A4 |
| ATOM | 1937 | CD1 | LEU | 289 | 44.604 | 7.179  | 35.378 | 1.00 | 0.00 | 3A4 |
| ATOM | 1938 | CD2 | LEU | 289 | 44.221 | 7.776  | 32.951 | 1.00 | 0.00 | 3A4 |
| ATOM | 1939 | C   | LEU | 289 | 46.475 | 4.056  | 32.878 | 1.00 | 0.00 | 3A4 |
| ATOM | 1940 | O   | LEU | 289 | 46.614 | 3.704  | 34.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 1941 | N   | SER | 290 | 46.131 | 3.176  | 31.880 | 1.00 | 0.00 | 3A4 |
| ATOM | 1942 | CA  | SER | 290 | 46.112 | 1.765  | 32.148 | 1.00 | 0.00 | 3A4 |
| ATOM | 1943 | CB  | SER | 290 | 45.026 | 1.325  | 33.179 | 1.00 | 0.00 | 3A4 |
| ATOM | 1944 | OG  | SER | 290 | 43.728 | 1.835  | 32.895 | 1.00 | 0.00 | 3A4 |
| ATOM | 1945 | C   | SER | 290 | 45.931 | 1.008  | 30.867 | 1.00 | 0.00 | 3A4 |
| ATOM | 1946 | O   | SER | 290 | 45.432 | 1.483  | 29.847 | 1.00 | 0.00 | 3A4 |
| ATOM | 1947 | N   | ASP | 291 | 46.293 | -0.287 | 30.944 | 1.00 | 0.00 | 3A4 |
| ATOM | 1948 | CA  | ASP | 291 | 46.226 | -1.223 | 29.856 | 1.00 | 0.00 | 3A4 |
| ATOM | 1949 | CB  | ASP | 291 | 46.894 | -2.555 | 30.218 | 1.00 | 0.00 | 3A4 |
| ATOM | 1950 | CG  | ASP | 291 | 48.385 | -2.331 | 30.513 | 1.00 | 0.00 | 3A4 |
| ATOM | 1951 | OD1 | ASP | 291 | 49.127 | -1.982 | 29.555 | 1.00 | 0.00 | 3A4 |
| ATOM | 1952 | OD2 | ASP | 291 | 48.800 | -2.508 | 31.690 | 1.00 | 0.00 | 3A4 |
| ATOM | 1953 | C   | ASP | 291 | 44.820 | -1.495 | 29.390 | 1.00 | 0.00 | 3A4 |
| ATOM | 1954 | O   | ASP | 291 | 44.578 | -1.735 | 28.227 | 1.00 | 0.00 | 3A4 |
| ATOM | 1955 | N   | LEU | 292 | 43.831 | -1.426 | 30.296 | 1.00 | 0.00 | 3A4 |
| ATOM | 1956 | CA  | LEU | 292 | 42.433 | -1.624 | 29.999 | 1.00 | 0.00 | 3A4 |
| ATOM | 1957 | CB  | LEU | 292 | 41.659 | -1.848 | 31.312 | 1.00 | 0.00 | 3A4 |
| ATOM | 1958 | CG  | LEU | 292 | 41.910 | -3.218 | 31.978 | 1.00 | 0.00 | 3A4 |
| ATOM | 1959 | CD1 | LEU | 292 | 41.502 | -3.197 | 33.463 | 1.00 | 0.00 | 3A4 |
| ATOM | 1960 | CD2 | LEU | 292 | 41.193 | -4.362 | 31.230 | 1.00 | 0.00 | 3A4 |
| ATOM | 1961 | C   | LEU | 292 | 41.827 | -0.445 | 29.268 | 1.00 | 0.00 | 3A4 |
| ATOM | 1962 | O   | LEU | 292 | 41.078 | -0.602 | 28.309 | 1.00 | 0.00 | 3A4 |
| ATOM | 1963 | N   | GLU | 293 | 42.216 | 0.784  | 29.669 | 1.00 | 0.00 | 3A4 |
| ATOM | 1964 | CA  | GLU | 293 | 41.794 | 2.025  | 29.064 | 1.00 | 0.00 | 3A4 |
| ATOM | 1965 | CB  | GLU | 293 | 42.258 | 3.233  | 29.892 | 1.00 | 0.00 | 3A4 |
| ATOM | 1966 | CG  | GLU | 293 | 41.403 | 3.396  | 31.163 | 1.00 | 0.00 | 3A4 |
| ATOM | 1967 | CD  | GLU | 293 | 41.950 | 4.520  | 32.046 | 1.00 | 0.00 | 3A4 |
| ATOM | 1968 | OE1 | GLU | 293 | 41.285 | 4.842  | 33.067 | 1.00 | 0.00 | 3A4 |
| ATOM | 1969 | OE2 | GLU | 293 | 43.037 | 5.066  | 31.722 | 1.00 | 0.00 | 3A4 |
| ATOM | 1970 | C   | GLU | 293 | 42.286 | 2.186  | 27.666 | 1.00 | 0.00 | 3A4 |
| ATOM | 1971 | O   | GLU | 293 | 41.540 | 2.607  | 26.793 | 1.00 | 0.00 | 3A4 |
| ATOM | 1972 | N   | LEU | 294 | 43.547 | 1.769  | 27.420 | 1.00 | 0.00 | 3A4 |
| ATOM | 1973 | CA  | LEU | 294 | 44.175 | 1.802  | 26.122 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 1974 | CB  | LEU | 294 | 45.633 | 1.380  | 26.208 | 1.00 | 0.00 | 3A4 |
| ATOM | 1975 | CG  | LEU | 294 | 46.091 | -0.086 | 26.051 | 1.00 | 0.00 | 3A4 |
| ATOM | 1976 | CD1 | LEU | 294 | 46.203 | -0.637 | 24.643 | 1.00 | 0.00 | 3A4 |
| ATOM | 1977 | CD2 | LEU | 294 | 47.365 | -0.436 | 26.810 | 1.00 | 0.00 | 3A4 |
| ATOM | 1978 | C   | LEU | 294 | 43.443 | 0.944  | 25.134 | 1.00 | 0.00 | 3A4 |
| ATOM | 1979 | O   | LEU | 294 | 43.172 | 1.361  | 24.020 | 1.00 | 0.00 | 3A4 |
| ATOM | 1980 | N   | VAL | 295 | 43.044 | -0.282 | 25.551 | 1.00 | 0.00 | 3A4 |
| ATOM | 1981 | CA  | VAL | 295 | 42.358 | -1.242 | 24.721 | 1.00 | 0.00 | 3A4 |
| ATOM | 1982 | CB  | VAL | 295 | 42.271 | -2.600 | 25.380 | 1.00 | 0.00 | 3A4 |
| ATOM | 1983 | CG1 | VAL | 295 | 41.397 | -3.622 | 24.599 | 1.00 | 0.00 | 3A4 |
| ATOM | 1984 | CG2 | VAL | 295 | 43.701 | -3.178 | 25.429 | 1.00 | 0.00 | 3A4 |
| ATOM | 1985 | C   | VAL | 295 | 40.980 | -0.762 | 24.357 | 1.00 | 0.00 | 3A4 |
| ATOM | 1986 | O   | VAL | 295 | 40.584 | -0.846 | 23.207 | 1.00 | 0.00 | 3A4 |
| ATOM | 1987 | N   | ALA | 296 | 40.252 | -0.146 | 25.306 | 1.00 | 0.00 | 3A4 |
| ATOM | 1988 | CA  | ALA | 296 | 38.945 | 0.439  | 25.074 | 1.00 | 0.00 | 3A4 |
| ATOM | 1989 | CB  | ALA | 296 | 38.344 | 0.902  | 26.408 | 1.00 | 0.00 | 3A4 |
| ATOM | 1990 | C   | ALA | 296 | 38.944 | 1.619  | 24.132 | 1.00 | 0.00 | 3A4 |
| ATOM | 1991 | O   | ALA | 296 | 38.032 | 1.797  | 23.342 | 1.00 | 0.00 | 3A4 |
| ATOM | 1992 | N   | GLN | 297 | 40.018 | 2.430  | 24.170 | 1.00 | 0.00 | 3A4 |
| ATOM | 1993 | CA  | GLN | 297 | 40.228 | 3.546  | 23.284 | 1.00 | 0.00 | 3A4 |
| ATOM | 1994 | CB  | GLN | 297 | 41.379 | 4.436  | 23.773 | 1.00 | 0.00 | 3A4 |
| ATOM | 1995 | CG  | GLN | 297 | 40.914 | 5.233  | 25.008 | 1.00 | 0.00 | 3A4 |
| ATOM | 1996 | CD  | GLN | 297 | 42.099 | 5.887  | 25.715 | 1.00 | 0.00 | 3A4 |
| ATOM | 1997 | OE1 | GLN | 297 | 43.052 | 5.222  | 26.114 | 1.00 | 0.00 | 3A4 |
| ATOM | 1998 | NE2 | GLN | 297 | 42.034 | 7.228  | 25.902 | 1.00 | 0.00 | 3A4 |
| ATOM | 1999 | C   | GLN | 297 | 40.505 | 3.108  | 21.882 | 1.00 | 0.00 | 3A4 |
| ATOM | 2000 | O   | GLN | 297 | 39.872 | 3.572  | 20.943 | 1.00 | 0.00 | 3A4 |
| ATOM | 2001 | N   | SER | 298 | 41.403 | 2.117  | 21.715 | 1.00 | 0.00 | 3A4 |
| ATOM | 2002 | CA  | SER | 298 | 41.744 | 1.546  | 20.434 | 1.00 | 0.00 | 3A4 |
| ATOM | 2003 | CB  | SER | 298 | 42.925 | 0.563  | 20.529 | 1.00 | 0.00 | 3A4 |
| ATOM | 2004 | OG  | SER | 298 | 42.771 | -0.519 | 21.435 | 1.00 | 0.00 | 3A4 |
| ATOM | 2005 | C   | SER | 298 | 40.584 | 0.872  | 19.755 | 1.00 | 0.00 | 3A4 |
| ATOM | 2006 | O   | SER | 298 | 40.435 | 0.977  | 18.546 | 1.00 | 0.00 | 3A4 |
| ATOM | 2007 | N   | ILE | 299 | 39.688 | 0.228  | 20.542 | 1.00 | 0.00 | 3A4 |
| ATOM | 2008 | CA  | ILE | 299 | 38.438 | -0.363 | 20.098 | 1.00 | 0.00 | 3A4 |
| ATOM | 2009 | CB  | ILE | 299 | 37.670 | -1.032 | 21.291 | 1.00 | 0.00 | 3A4 |
| ATOM | 2010 | CG2 | ILE | 299 | 36.134 | -1.268 | 21.098 | 1.00 | 0.00 | 3A4 |
| ATOM | 2011 | CG1 | ILE | 299 | 38.328 | -2.333 | 21.803 | 1.00 | 0.00 | 3A4 |
| ATOM | 2012 | CD  | ILE | 299 | 37.787 | -3.619 | 21.185 | 1.00 | 0.00 | 3A4 |
| ATOM | 2013 | C   | ILE | 299 | 37.515 | 0.677  | 19.534 | 1.00 | 0.00 | 3A4 |
| ATOM | 2014 | O   | ILE | 299 | 36.949 | 0.525  | 18.457 | 1.00 | 0.00 | 3A4 |
| ATOM | 2015 | N   | ILE | 300 | 37.374 | 1.799  | 20.268 | 1.00 | 0.00 | 3A4 |
| ATOM | 2016 | CA  | ILE | 300 | 36.494 | 2.883  | 19.921 | 1.00 | 0.00 | 3A4 |
| ATOM | 2017 | CB  | ILE | 300 | 36.290 | 3.798  | 21.113 | 1.00 | 0.00 | 3A4 |
| ATOM | 2018 | CG2 | ILE | 300 | 36.292 | 5.340  | 20.897 | 1.00 | 0.00 | 3A4 |
| ATOM | 2019 | CG1 | ILE | 300 | 34.906 | 3.296  | 21.637 | 1.00 | 0.00 | 3A4 |
| ATOM | 2020 | CD  | ILE | 300 | 34.503 | 3.642  | 23.050 | 1.00 | 0.00 | 3A4 |
| ATOM | 2021 | C   | ILE | 300 | 36.962 | 3.618  | 18.712 | 1.00 | 0.00 | 3A4 |
| ATOM | 2022 | O   | ILE | 300 | 36.161 | 3.994  | 17.872 | 1.00 | 0.00 | 3A4 |
| ATOM | 2023 | N   | PHE | 301 | 38.279 | 3.774  | 18.515 | 1.00 | 0.00 | 3A4 |
| ATOM | 2024 | CA  | PHE | 301 | 38.819 | 4.525  | 17.406 | 1.00 | 0.00 | 3A4 |
| ATOM | 2025 | CB  | PHE | 301 | 40.332 | 4.745  | 17.663 | 1.00 | 0.00 | 3A4 |
| ATOM | 2026 | CG  | PHE | 301 | 40.520 | 5.958  | 18.535 | 1.00 | 0.00 | 3A4 |
| ATOM | 2027 | CD1 | PHE | 301 | 41.157 | 5.931  | 19.784 | 1.00 | 0.00 | 3A4 |
| ATOM | 2028 | CD2 | PHE | 301 | 39.913 | 7.144  | 18.106 | 1.00 | 0.00 | 3A4 |
| ATOM | 2029 | CE1 | PHE | 301 | 41.032 | 7.015  | 20.660 | 1.00 | 0.00 | 3A4 |
| ATOM | 2030 | CE2 | PHE | 301 | 39.784 | 8.213  | 18.969 | 1.00 | 0.00 | 3A4 |
| ATOM | 2031 | CZ  | PHE | 301 | 40.300 | 8.142  | 20.259 | 1.00 | 0.00 | 3A4 |
| ATOM | 2032 | C   | PHE | 301 | 38.633 | 3.743  | 16.111 | 1.00 | 0.00 | 3A4 |
| ATOM | 2033 | O   | PHE | 301 | 38.332 | 4.306  | 15.062 | 1.00 | 0.00 | 3A4 |
| ATOM | 2034 | N   | ILE | 302 | 38.742 | 2.401  | 16.178 | 1.00 | 0.00 | 3A4 |
| ATOM | 2035 | CA  | ILE | 302 | 38.511 | 1.491  | 15.076 | 1.00 | 0.00 | 3A4 |
| ATOM | 2036 | CB  | ILE | 302 | 39.005 | 0.104  | 15.470 | 1.00 | 0.00 | 3A4 |
| ATOM | 2037 | CG2 | ILE | 302 | 38.482 | -1.056 | 14.570 | 1.00 | 0.00 | 3A4 |
| ATOM | 2038 | CG1 | ILE | 302 | 40.563 | 0.105  | 15.527 | 1.00 | 0.00 | 3A4 |
| ATOM | 2039 | CD  | ILE | 302 | 41.293 | 0.195  | 14.178 | 1.00 | 0.00 | 3A4 |
| ATOM | 2040 | C   | ILE | 302 | 37.054 | 1.462  | 14.656 | 1.00 | 0.00 | 3A4 |
| ATOM | 2041 | O   | ILE | 302 | 36.732 | 1.682  | 13.491 | 1.00 | 0.00 | 3A4 |
| ATOM | 2042 | N   | PHE | 303 | 36.126 | 1.231  | 15.610 | 1.00 | 0.00 | 3A4 |
| ATOM | 2043 | CA  | PHE | 303 | 34.711 | 1.090  | 15.324 | 1.00 | 0.00 | 3A4 |
| ATOM | 2044 | CB  | PHE | 303 | 34.008 | 0.159  | 16.395 | 1.00 | 0.00 | 3A4 |
| ATOM | 2045 | CG  | PHE | 303 | 33.072 | 0.735  | 17.449 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2046 | CD1 | PHE | 303 | 31.783 | 1.209  | 17.127 | 1.00 | 0.00 | 3A4 |
| ATOM | 2047 | CD2 | PHE | 303 | 33.443 | 0.706  | 18.808 | 1.00 | 0.00 | 3A4 |
| ATOM | 2048 | CE1 | PHE | 303 | 30.911 | 1.674  | 18.121 | 1.00 | 0.00 | 3A4 |
| ATOM | 2049 | CE2 | PHE | 303 | 32.572 | 1.155  | 19.810 | 1.00 | 0.00 | 3A4 |
| ATOM | 2050 | CZ  | PHE | 303 | 31.307 | 1.647  | 19.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 2051 | C   | PHE | 303 | 34.016 | 2.407  | 14.993 | 1.00 | 0.00 | 3A4 |
| ATOM | 2052 | O   | PHE | 303 | 33.183 | 2.472  | 14.092 | 1.00 | 0.00 | 3A4 |
| ATOM | 2053 | N   | ALA | 304 | 34.391 | 3.513  | 15.679 | 1.00 | 0.00 | 3A4 |
| ATOM | 2054 | CA  | ALA | 304 | 33.814 | 4.831  | 15.484 | 1.00 | 0.00 | 3A4 |
| ATOM | 2055 | CB  | ALA | 304 | 34.124 | 5.826  | 16.638 | 1.00 | 0.00 | 3A4 |
| ATOM | 2056 | C   | ALA | 304 | 34.221 | 5.470  | 14.208 | 1.00 | 0.00 | 3A4 |
| ATOM | 2057 | O   | ALA | 304 | 33.449 | 6.196  | 13.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 2058 | N   | GLY | 305 | 35.466 | 5.191  | 13.787 | 1.00 | 0.00 | 3A4 |
| ATOM | 2059 | CA  | GLY | 305 | 36.037 | 5.755  | 12.599 | 1.00 | 0.00 | 3A4 |
| ATOM | 2060 | C   | GLY | 305 | 35.766 | 5.044  | 11.304 | 1.00 | 0.00 | 3A4 |
| ATOM | 2061 | O   | GLY | 305 | 36.028 | 5.603  | 10.243 | 1.00 | 0.00 | 3A4 |
| ATOM | 2062 | N   | TYR | 306 | 35.257 | 3.789  | 11.337 | 1.00 | 0.00 | 3A4 |
| ATOM | 2063 | CA  | TYR | 306 | 35.125 | 2.982  | 10.139 | 1.00 | 0.00 | 3A4 |
| ATOM | 2064 | CB  | TYR | 306 | 35.531 | 1.484  | 10.389 | 1.00 | 0.00 | 3A4 |
| ATOM | 2065 | CG  | TYR | 306 | 35.403 | 0.528  | 9.206  | 1.00 | 0.00 | 3A4 |
| ATOM | 2066 | CD1 | TYR | 306 | 35.378 | 0.950  | 7.858  | 1.00 | 0.00 | 3A4 |
| ATOM | 2067 | CD2 | TYR | 306 | 35.195 | -0.835 | 9.469  | 1.00 | 0.00 | 3A4 |
| ATOM | 2068 | CE1 | TYR | 306 | 35.009 | 0.064  | 6.843  | 1.00 | 0.00 | 3A4 |
| ATOM | 2069 | CE2 | TYR | 306 | 34.885 | -1.738 | 8.441  | 1.00 | 0.00 | 3A4 |
| ATOM | 2070 | CZ  | TYR | 306 | 34.766 | -1.281 | 7.125  | 1.00 | 0.00 | 3A4 |
| ATOM | 2071 | OH  | TYR | 306 | 34.383 | -2.159 | 6.089  | 1.00 | 0.00 | 3A4 |
| ATOM | 2072 | C   | TYR | 306 | 33.741 | 3.132  | 9.572  | 1.00 | 0.00 | 3A4 |
| ATOM | 2073 | O   | TYR | 306 | 33.566 | 3.553  | 8.431  | 1.00 | 0.00 | 3A4 |
| ATOM | 2074 | N   | GLU | 307 | 32.692 | 2.781  | 10.344 | 1.00 | 0.00 | 3A4 |
| ATOM | 2075 | CA  | GLU | 307 | 31.384 | 2.639  | 9.745  | 1.00 | 0.00 | 3A4 |
| ATOM | 2076 | CB  | GLU | 307 | 30.517 | 1.553  | 10.437 | 1.00 | 0.00 | 3A4 |
| ATOM | 2077 | CG  | GLU | 307 | 31.119 | 0.127  | 10.329 | 1.00 | 0.00 | 3A4 |
| ATOM | 2078 | CD  | GLU | 307 | 31.130 | -0.460 | 8.905  | 1.00 | 0.00 | 3A4 |
| ATOM | 2079 | OE1 | GLU | 307 | 30.600 | 0.159  | 7.942  | 1.00 | 0.00 | 3A4 |
| ATOM | 2080 | OE2 | GLU | 307 | 31.670 | -1.592 | 8.778  | 1.00 | 0.00 | 3A4 |
| ATOM | 2081 | C   | GLU | 307 | 30.630 | 3.933  | 9.563  | 1.00 | 0.00 | 3A4 |
| ATOM | 2082 | O   | GLU | 307 | 29.605 | 3.926  | 8.924  | 1.00 | 0.00 | 3A4 |
| ATOM | 2083 | N   | THR | 308 | 31.140 | 5.089  | 10.026 | 1.00 | 0.00 | 3A4 |
| ATOM | 2084 | CA  | THR | 308 | 30.556 | 6.394  | 9.788  | 1.00 | 0.00 | 3A4 |
| ATOM | 2085 | CB  | THR | 308 | 30.866 | 7.363  | 10.932 | 1.00 | 0.00 | 3A4 |
| ATOM | 2086 | OG1 | THR | 308 | 32.255 | 7.423  | 11.254 | 1.00 | 0.00 | 3A4 |
| ATOM | 2087 | CG2 | THR | 308 | 30.088 | 6.935  | 12.191 | 1.00 | 0.00 | 3A4 |
| ATOM | 2088 | C   | THR | 308 | 31.006 | 6.957  | 8.463  | 1.00 | 0.00 | 3A4 |
| ATOM | 2089 | O   | THR | 308 | 30.202 | 7.360  | 7.632  | 1.00 | 0.00 | 3A4 |
| ATOM | 2090 | N   | THR | 309 | 32.332 | 6.929  | 8.226  | 1.00 | 0.00 | 3A4 |
| ATOM | 2091 | CA  | THR | 309 | 32.979 | 7.436  | 7.038  | 1.00 | 0.00 | 3A4 |
| ATOM | 2092 | CB  | THR | 309 | 34.479 | 7.445  | 7.204  | 1.00 | 0.00 | 3A4 |
| ATOM | 2093 | OG1 | THR | 309 | 34.937 | 6.213  | 7.743  | 1.00 | 0.00 | 3A4 |
| ATOM | 2094 | CG2 | THR | 309 | 34.867 | 8.555  | 8.200  | 1.00 | 0.00 | 3A4 |
| ATOM | 2095 | C   | THR | 309 | 32.600 | 6.684  | 5.779  | 1.00 | 0.00 | 3A4 |
| ATOM | 2096 | O   | THR | 309 | 32.349 | 7.278  | 4.741  | 1.00 | 0.00 | 3A4 |
| ATOM | 2097 | N   | SER | 310 | 32.484 | 5.339  | 5.875  | 1.00 | 0.00 | 3A4 |
| ATOM | 2098 | CA  | SER | 310 | 32.052 | 4.458  | 4.809  | 1.00 | 0.00 | 3A4 |
| ATOM | 2099 | CB  | SER | 310 | 31.996 | 2.990  | 5.310  | 1.00 | 0.00 | 3A4 |
| ATOM | 2100 | OG  | SER | 310 | 33.306 | 2.563  | 5.646  | 1.00 | 0.00 | 3A4 |
| ATOM | 2101 | C   | SER | 310 | 30.666 | 4.763  | 4.322  | 1.00 | 0.00 | 3A4 |
| ATOM | 2102 | O   | SER | 310 | 30.413 | 4.886  | 3.131  | 1.00 | 0.00 | 3A4 |
| ATOM | 2103 | N   | SER | 311 | 29.728 | 4.960  | 5.261  | 1.00 | 0.00 | 3A4 |
| ATOM | 2104 | CA  | SER | 311 | 28.351 | 5.245  | 4.950  | 1.00 | 0.00 | 3A4 |
| ATOM | 2105 | CB  | SER | 311 | 27.509 | 5.056  | 6.222  | 1.00 | 0.00 | 3A4 |
| ATOM | 2106 | OG  | SER | 311 | 27.701 | 3.739  | 6.719  | 1.00 | 0.00 | 3A4 |
| ATOM | 2107 | C   | SER | 311 | 28.153 | 6.627  | 4.389  | 1.00 | 0.00 | 3A4 |
| ATOM | 2108 | O   | SER | 311 | 27.316 | 6.833  | 3.523  | 1.00 | 0.00 | 3A4 |
| ATOM | 2109 | N   | VAL | 312 | 28.984 | 7.609  | 4.813  | 1.00 | 0.00 | 3A4 |
| ATOM | 2110 | CA  | VAL | 312 | 28.964 | 8.970  | 4.310  | 1.00 | 0.00 | 3A4 |
| ATOM | 2111 | CB  | VAL | 312 | 29.781 | 9.902  | 5.173  | 1.00 | 0.00 | 3A4 |
| ATOM | 2112 | CG1 | VAL | 312 | 29.980 | 11.315 | 4.570  | 1.00 | 0.00 | 3A4 |
| ATOM | 2113 | CG2 | VAL | 312 | 28.894 | 10.077 | 6.433  | 1.00 | 0.00 | 3A4 |
| ATOM | 2114 | C   | VAL | 312 | 29.408 | 9.072  | 2.884  | 1.00 | 0.00 | 3A4 |
| ATOM | 2115 | O   | VAL | 312 | 28.751 | 9.739  | 2.103  | 1.00 | 0.00 | 3A4 |
| ATOM | 2116 | N   | LEU | 313 | 30.463 | 8.328  | 2.495  | 1.00 | 0.00 | 3A4 |
| ATOM | 2117 | CA  | LEU | 313 | 30.996 | 8.277  | 1.150  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2118 | CB  | LEU | 313 | 32.294 | 7.466  | 1.085  | 1.00 | 0.00 | 3A4 |
| ATOM | 2119 | CG  | LEU | 313 | 33.512 | 8.219  | 1.649  | 1.00 | 0.00 | 3A4 |
| ATOM | 2120 | CD1 | LEU | 313 | 34.492 | 8.511  | 0.499  | 1.00 | 0.00 | 3A4 |
| ATOM | 2121 | CD2 | LEU | 313 | 33.322 | 9.485  | 2.496  | 1.00 | 0.00 | 3A4 |
| ATOM | 2122 | C   | LEU | 313 | 30.017 | 7.696  | 0.167  | 1.00 | 0.00 | 3A4 |
| ATOM | 2123 | O   | LEU | 313 | 29.808 | 8.229  | -0.917 | 1.00 | 0.00 | 3A4 |
| ATOM | 2124 | N   | SER | 314 | 29.309 | 6.624  | 0.579  | 1.00 | 0.00 | 3A4 |
| ATOM | 2125 | CA  | SER | 314 | 28.305 | 5.981  | -0.243 | 1.00 | 0.00 | 3A4 |
| ATOM | 2126 | CB  | SER | 314 | 27.992 | 4.570  | 0.299  | 1.00 | 0.00 | 3A4 |
| ATOM | 2127 | OG  | SER | 314 | 29.195 | 3.821  | 0.397  | 1.00 | 0.00 | 3A4 |
| ATOM | 2128 | C   | SER | 314 | 27.070 | 6.845  | -0.420 | 1.00 | 0.00 | 3A4 |
| ATOM | 2129 | O   | SER | 314 | 26.505 | 6.909  | -1.507 | 1.00 | 0.00 | 3A4 |
| ATOM | 2130 | N   | PHE | 315 | 26.702 | 7.636  | 0.625  | 1.00 | 0.00 | 3A4 |
| ATOM | 2131 | CA  | PHE | 315 | 25.595 | 8.572  | 0.583  | 1.00 | 0.00 | 3A4 |
| ATOM | 2132 | CB  | PHE | 315 | 25.181 | 9.076  | 2.015  | 1.00 | 0.00 | 3A4 |
| ATOM | 2133 | CG  | PHE | 315 | 23.897 | 8.407  | 2.456  | 1.00 | 0.00 | 3A4 |
| ATOM | 2134 | CD1 | PHE | 315 | 23.856 | 7.678  | 3.662  | 1.00 | 0.00 | 3A4 |
| ATOM | 2135 | CD2 | PHE | 315 | 22.732 | 8.451  | 1.660  | 1.00 | 0.00 | 3A4 |
| ATOM | 2136 | CE1 | PHE | 315 | 22.683 | 7.024  | 4.067  | 1.00 | 0.00 | 3A4 |
| ATOM | 2137 | CE2 | PHE | 315 | 21.568 | 7.770  | 2.047  | 1.00 | 0.00 | 3A4 |
| ATOM | 2138 | CZ  | PHE | 315 | 21.542 | 7.061  | 3.254  | 1.00 | 0.00 | 3A4 |
| ATOM | 2139 | C   | PHE | 315 | 25.938 | 9.760  | -0.291 | 1.00 | 0.00 | 3A4 |
| ATOM | 2140 | O   | PHE | 315 | 25.075 | 10.250 | -1.011 | 1.00 | 0.00 | 3A4 |
| ATOM | 2141 | N   | ILE | 316 | 27.230 | 10.200 | -0.328 | 1.00 | 0.00 | 3A4 |
| ATOM | 2142 | CA  | ILE | 316 | 27.669 | 11.286 | -1.202 | 1.00 | 0.00 | 3A4 |
| ATOM | 2143 | CB  | ILE | 316 | 29.119 | 11.864 | -1.060 | 1.00 | 0.00 | 3A4 |
| ATOM | 2144 | CG2 | ILE | 316 | 29.128 | 13.291 | -1.688 | 1.00 | 0.00 | 3A4 |
| ATOM | 2145 | CG1 | ILE | 316 | 29.687 | 11.833 | 0.371  | 1.00 | 0.00 | 3A4 |
| ATOM | 2146 | CD  | ILE | 316 | 30.950 | 12.629 | 0.687  | 1.00 | 0.00 | 3A4 |
| ATOM | 2147 | C   | ILE | 316 | 27.559 | 10.926 | -2.666 | 1.00 | 0.00 | 3A4 |
| ATOM | 2148 | O   | ILE | 316 | 27.111 | 11.726 | -3.476 | 1.00 | 0.00 | 3A4 |
| ATOM | 2149 | N   | MET | 317 | 27.919 | 9.671  | -3.009 | 1.00 | 0.00 | 3A4 |
| ATOM | 2150 | CA  | MET | 317 | 27.868 | 9.137  | -4.351 | 1.00 | 0.00 | 3A4 |
| ATOM | 2151 | CB  | MET | 317 | 28.640 | 7.803  | -4.441 | 1.00 | 0.00 | 3A4 |
| ATOM | 2152 | CG  | MET | 317 | 30.148 | 8.007  | -4.191 | 1.00 | 0.00 | 3A4 |
| ATOM | 2153 | SD  | MET | 317 | 31.027 | 6.548  | -3.550 | 1.00 | 0.00 | 3A4 |
| ATOM | 2154 | CE  | MET | 317 | 32.475 | 7.489  | -2.987 | 1.00 | 0.00 | 3A4 |
| ATOM | 2155 | C   | MET | 317 | 26.449 | 8.978  | -4.853 | 1.00 | 0.00 | 3A4 |
| ATOM | 2156 | O   | MET | 317 | 26.139 | 9.327  | -5.986 | 1.00 | 0.00 | 3A4 |
| ATOM | 2157 | N   | TYR | 318 | 25.516 | 8.539  | -3.981 | 1.00 | 0.00 | 3A4 |
| ATOM | 2158 | CA  | TYR | 318 | 24.101 | 8.458  | -4.293 | 1.00 | 0.00 | 3A4 |
| ATOM | 2159 | CB  | TYR | 318 | 23.333 | 7.794  | -3.134 | 1.00 | 0.00 | 3A4 |
| ATOM | 2160 | CG  | TYR | 318 | 21.822 | 7.683  | -3.312 | 1.00 | 0.00 | 3A4 |
| ATOM | 2161 | CD1 | TYR | 318 | 21.269 | 7.039  | -4.436 | 1.00 | 0.00 | 3A4 |
| ATOM | 2162 | CD2 | TYR | 318 | 20.950 | 8.269  | -2.372 | 1.00 | 0.00 | 3A4 |
| ATOM | 2163 | CE1 | TYR | 318 | 19.881 | 6.987  | -4.624 | 1.00 | 0.00 | 3A4 |
| ATOM | 2164 | CE2 | TYR | 318 | 19.560 | 8.209  | -2.548 | 1.00 | 0.00 | 3A4 |
| ATOM | 2165 | CZ  | TYR | 318 | 19.024 | 7.566  | -3.675 | 1.00 | 0.00 | 3A4 |
| ATOM | 2166 | OH  | TYR | 318 | 17.625 | 7.498  | -3.855 | 1.00 | 0.00 | 3A4 |
| ATOM | 2167 | C   | TYR | 318 | 23.501 | 9.814  | -4.592 | 1.00 | 0.00 | 3A4 |
| ATOM | 2168 | O   | TYR | 318 | 22.759 | 9.967  | -5.553 | 1.00 | 0.00 | 3A4 |
| ATOM | 2169 | N   | GLU | 319 | 23.864 | 10.847 | -3.796 | 1.00 | 0.00 | 3A4 |
| ATOM | 2170 | CA  | GLU | 319 | 23.389 | 12.203 | -3.970 | 1.00 | 0.00 | 3A4 |
| ATOM | 2171 | CB  | GLU | 319 | 23.703 | 13.127 | -2.775 | 1.00 | 0.00 | 3A4 |
| ATOM | 2172 | CG  | GLU | 319 | 22.849 | 12.760 | -1.559 | 1.00 | 0.00 | 3A4 |
| ATOM | 2173 | CD  | GLU | 319 | 23.038 | 13.838 | -0.506 | 1.00 | 0.00 | 3A4 |
| ATOM | 2174 | OE1 | GLU | 319 | 24.202 | 14.049 | -0.085 | 1.00 | 0.00 | 3A4 |
| ATOM | 2175 | OE2 | GLU | 319 | 22.027 | 14.476 | -0.119 | 1.00 | 0.00 | 3A4 |
| ATOM | 2176 | C   | GLU | 319 | 23.894 | 12.847 | -5.231 | 1.00 | 0.00 | 3A4 |
| ATOM | 2177 | O   | GLU | 319 | 23.132 | 13.474 | -5.951 | 1.00 | 0.00 | 3A4 |
| ATOM | 2178 | N   | LEU | 320 | 25.170 | 12.641 | -5.595 | 1.00 | 0.00 | 3A4 |
| ATOM | 2179 | CA  | LEU | 320 | 25.713 | 13.161 | -6.828 | 1.00 | 0.00 | 3A4 |
| ATOM | 2180 | CB  | LEU | 320 | 27.239 | 13.059 | -6.841 | 1.00 | 0.00 | 3A4 |
| ATOM | 2181 | CG  | LEU | 320 | 27.880 | 14.027 | -5.843 | 1.00 | 0.00 | 3A4 |
| ATOM | 2182 | CD1 | LEU | 320 | 29.380 | 13.757 | -5.709 | 1.00 | 0.00 | 3A4 |
| ATOM | 2183 | CD2 | LEU | 320 | 27.611 | 15.489 | -6.192 | 1.00 | 0.00 | 3A4 |
| ATOM | 2184 | C   | LEU | 320 | 25.160 | 12.475 | -8.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 2185 | O   | LEU | 320 | 24.977 | 13.105 | -9.083 | 1.00 | 0.00 | 3A4 |
| ATOM | 2186 | N   | ALA | 321 | 24.818 | 11.177 | -7.933 | 1.00 | 0.00 | 3A4 |
| ATOM | 2187 | CA  | ALA | 321 | 24.215 | 10.397 | -8.990 | 1.00 | 0.00 | 3A4 |
| ATOM | 2188 | CB  | ALA | 321 | 24.217 | 8.897  | -8.645 | 1.00 | 0.00 | 3A4 |
| ATOM | 2189 | C   | ALA | 321 | 22.802 | 10.861 | -9.259 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 2190 | O   | ALA | 321 | 22.338 | 10.884 | -10.397 | 1.00 | 0.00 | 3A4 |
| ATOM | 2191 | N   | THR | 322 | 22.103 | 11.305 | -8.194  | 1.00 | 0.00 | 3A4 |
| ATOM | 2192 | CA  | THR | 322 | 20.743 | 11.780 | -8.258  | 1.00 | 0.00 | 3A4 |
| ATOM | 2193 | CB  | THR | 322 | 19.981 | 11.519 | -6.972  | 1.00 | 0.00 | 3A4 |
| ATOM | 2194 | OG1 | THR | 322 | 20.610 | 11.999 | -5.794  | 1.00 | 0.00 | 3A4 |
| ATOM | 2195 | CG2 | THR | 322 | 19.745 | 9.994  | -6.849  | 1.00 | 0.00 | 3A4 |
| ATOM | 2196 | C   | THR | 322 | 20.627 | 13.242 | -8.642  | 1.00 | 0.00 | 3A4 |
| ATOM | 2197 | O   | THR | 322 | 19.555 | 13.704 | -9.018  | 1.00 | 0.00 | 3A4 |
| ATOM | 2198 | N   | HIS | 323 | 21.731 | 14.006 | -8.558  | 1.00 | 0.00 | 3A4 |
| ATOM | 2199 | CA  | HIS | 323 | 21.740 | 15.416 | -8.856  | 1.00 | 0.00 | 3A4 |
| ATOM | 2200 | ND1 | HIS | 323 | 20.544 | 15.212 | -5.650  | 1.00 | 0.00 | 3A4 |
| ATOM | 2201 | CG  | HIS | 323 | 20.676 | 16.147 | -6.653  | 1.00 | 0.00 | 3A4 |
| ATOM | 2202 | CB  | HIS | 323 | 21.859 | 16.259 | -7.581  | 1.00 | 0.00 | 3A4 |
| ATOM | 2203 | NE2 | HIS | 323 | 18.715 | 16.470 | -5.582  | 1.00 | 0.00 | 3A4 |
| ATOM | 2204 | CD2 | HIS | 323 | 19.549 | 16.908 | -6.595  | 1.00 | 0.00 | 3A4 |
| ATOM | 2205 | CE1 | HIS | 323 | 19.356 | 15.449 | -5.043  | 1.00 | 0.00 | 3A4 |
| ATOM | 2206 | C   | HIS | 323 | 22.892 | 15.711 | -9.775  | 1.00 | 0.00 | 3A4 |
| ATOM | 2207 | O   | HIS | 323 | 23.883 | 16.309 | -9.352  | 1.00 | 0.00 | 3A4 |
| ATOM | 2208 | N   | PRO | 324 | 22.833 | 15.378 | -11.076 | 1.00 | 0.00 | 3A4 |
| ATOM | 2209 | CA  | PRO | 324 | 23.958 | 15.508 | -12.002 | 1.00 | 0.00 | 3A4 |
| ATOM | 2210 | CD  | PRO | 324 | 21.602 | 14.983 | -11.765 | 1.00 | 0.00 | 3A4 |
| ATOM | 2211 | CB  | PRO | 324 | 23.420 | 14.910 | -13.300 | 1.00 | 0.00 | 3A4 |
| ATOM | 2212 | CG  | PRO | 324 | 21.905 | 15.129 | -13.255 | 1.00 | 0.00 | 3A4 |
| ATOM | 2213 | C   | PRO | 324 | 24.415 | 16.938 | -12.213 | 1.00 | 0.00 | 3A4 |
| ATOM | 2214 | O   | PRO | 324 | 25.575 | 17.158 | -12.534 | 1.00 | 0.00 | 3A4 |
| ATOM | 2215 | N   | ASP | 325 | 23.561 | 17.950 | -11.949 | 1.00 | 0.00 | 3A4 |
| ATOM | 2216 | CA  | ASP | 325 | 23.917 | 19.351 | -12.002 | 1.00 | 0.00 | 3A4 |
| ATOM | 2217 | CB  | ASP | 325 | 22.668 | 20.245 | -11.821 | 1.00 | 0.00 | 3A4 |
| ATOM | 2218 | CG  | ASP | 325 | 21.653 | 19.933 | -12.931 | 1.00 | 0.00 | 3A4 |
| ATOM | 2219 | OD1 | ASP | 325 | 21.991 | 20.159 | -14.125 | 1.00 | 0.00 | 3A4 |
| ATOM | 2220 | OD2 | ASP | 325 | 20.531 | 19.463 | -12.600 | 1.00 | 0.00 | 3A4 |
| ATOM | 2221 | C   | ASP | 325 | 24.927 | 19.731 | -10.944 | 1.00 | 0.00 | 3A4 |
| ATOM | 2222 | O   | ASP | 325 | 25.817 | 20.547 | -11.169 | 1.00 | 0.00 | 3A4 |
| ATOM | 2223 | N   | VAL | 326 | 24.835 | 19.071 | -9.767  | 1.00 | 0.00 | 3A4 |
| ATOM | 2224 | CA  | VAL | 326 | 25.742 | 19.249 | -8.647  | 1.00 | 0.00 | 3A4 |
| ATOM | 2225 | CB  | VAL | 326 | 25.198 | 18.672 | -7.341  | 1.00 | 0.00 | 3A4 |
| ATOM | 2226 | CG1 | VAL | 326 | 26.201 | 18.872 | -6.173  | 1.00 | 0.00 | 3A4 |
| ATOM | 2227 | CG2 | VAL | 326 | 23.874 | 19.402 | -7.034  | 1.00 | 0.00 | 3A4 |
| ATOM | 2228 | C   | VAL | 326 | 27.083 | 18.648 | -8.960  | 1.00 | 0.00 | 3A4 |
| ATOM | 2229 | O   | VAL | 326 | 28.106 | 19.288 | -8.782  | 1.00 | 0.00 | 3A4 |
| ATOM | 2230 | N   | GLN | 327 | 27.089 | 17.427 | -9.528  | 1.00 | 0.00 | 3A4 |
| ATOM | 2231 | CA  | GLN | 327 | 28.281 | 16.718 | -9.931  | 1.00 | 0.00 | 3A4 |
| ATOM | 2232 | CB  | GLN | 327 | 27.899 | 15.340 | -10.487 | 1.00 | 0.00 | 3A4 |
| ATOM | 2233 | CG  | GLN | 327 | 29.062 | 14.350 | -10.683 | 1.00 | 0.00 | 3A4 |
| ATOM | 2234 | CD  | GLN | 327 | 28.538 | 12.991 | -11.166 | 1.00 | 0.00 | 3A4 |
| ATOM | 2235 | OE1 | GLN | 327 | 27.336 | 12.728 | -11.186 | 1.00 | 0.00 | 3A4 |
| ATOM | 2236 | NE2 | GLN | 327 | 29.475 | 12.091 | -11.572 | 1.00 | 0.00 | 3A4 |
| ATOM | 2237 | C   | GLN | 327 | 29.088 | 17.459 | -10.960 | 1.00 | 0.00 | 3A4 |
| ATOM | 2238 | O   | GLN | 327 | 30.301 | 17.551 | -10.855 | 1.00 | 0.00 | 3A4 |
| ATOM | 2239 | N   | GLN | 328 | 28.408 | 18.092 | -11.941 | 1.00 | 0.00 | 3A4 |
| ATOM | 2240 | CA  | GLN | 328 | 29.023 | 18.879 | -12.995 | 1.00 | 0.00 | 3A4 |
| ATOM | 2241 | CB  | GLN | 328 | 27.977 | 19.321 | -14.041 | 1.00 | 0.00 | 3A4 |
| ATOM | 2242 | CG  | GLN | 328 | 27.544 | 18.163 | -14.957 | 1.00 | 0.00 | 3A4 |
| ATOM | 2243 | CD  | GLN | 328 | 26.423 | 18.643 | -15.885 | 1.00 | 0.00 | 3A4 |
| ATOM | 2244 | OE1 | GLN | 328 | 26.675 | 19.426 | -16.800 | 1.00 | 0.00 | 3A4 |
| ATOM | 2245 | NE2 | GLN | 328 | 25.164 | 18.178 | -15.654 | 1.00 | 0.00 | 3A4 |
| ATOM | 2246 | C   | GLN | 328 | 29.711 | 20.106 | -12.470 | 1.00 | 0.00 | 3A4 |
| ATOM | 2247 | O   | GLN | 328 | 30.827 | 20.429 | -12.855 | 1.00 | 0.00 | 3A4 |
| ATOM | 2248 | N   | LYS | 329 | 29.068 | 20.782 | -11.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 2249 | CA  | LYS | 329 | 29.597 | 21.931 | -10.807 | 1.00 | 0.00 | 3A4 |
| ATOM | 2250 | CB  | LYS | 329 | 28.515 | 22.465 | -9.850  | 1.00 | 0.00 | 3A4 |
| ATOM | 2251 | CG  | LYS | 329 | 28.752 | 23.857 | -9.250  | 1.00 | 0.00 | 3A4 |
| ATOM | 2252 | CD  | LYS | 329 | 27.533 | 24.347 | -8.460  | 1.00 | 0.00 | 3A4 |
| ATOM | 2253 | CE  | LYS | 329 | 27.679 | 25.785 | -7.953  | 1.00 | 0.00 | 3A4 |
| ATOM | 2254 | NZ  | LYS | 329 | 26.477 | 26.210 | -7.202  | 1.00 | 0.00 | 3A4 |
| ATOM | 2255 | C   | LYS | 329 | 30.884 | 21.621 | -10.052 | 1.00 | 0.00 | 3A4 |
| ATOM | 2256 | O   | LYS | 329 | 31.860 | 22.366 | -10.101 | 1.00 | 0.00 | 3A4 |
| ATOM | 2257 | N   | LEU | 330 | 30.952 | 20.423 | -9.426  | 1.00 | 0.00 | 3A4 |
| ATOM | 2258 | CA  | LEU | 330 | 32.100 | 19.968 | -8.670  | 1.00 | 0.00 | 3A4 |
| ATOM | 2259 | CB  | LEU | 330 | 31.814 | 18.742 | -7.797  | 1.00 | 0.00 | 3A4 |
| ATOM | 2260 | CG  | LEU | 330 | 30.502 | 18.756 | -7.038  | 1.00 | 0.00 | 3A4 |
| ATOM | 2261 | CD1 | LEU | 330 | 30.541 | 17.732 | -5.920  | 1.00 | 0.00 | 3A4 |



|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 2262 | CD2 | LEU | 330 | 29.986 | 20.145 | -6.584  | 1.00 | 0.00 | 3A4 |
| ATOM | 2263 | C   | LEU | 330 | 33.250 | 19.598 | -9.579  | 1.00 | 0.00 | 3A4 |
| ATOM | 2264 | O   | LEU | 330 | 34.410 | 19.864 | -9.296  | 1.00 | 0.00 | 3A4 |
| ATOM | 2265 | N   | GLN | 331 | 32.931 | 18.993 | -10.741 | 1.00 | 0.00 | 3A4 |
| ATOM | 2266 | CA  | GLN | 331 | 33.881 | 18.627 | -11.762 | 1.00 | 0.00 | 3A4 |
| ATOM | 2267 | CB  | GLN | 331 | 33.229 | 17.787 | -12.880 | 1.00 | 0.00 | 3A4 |
| ATOM | 2268 | CG  | GLN | 331 | 32.942 | 16.354 | -12.389 | 1.00 | 0.00 | 3A4 |
| ATOM | 2269 | CD  | GLN | 331 | 32.147 | 15.568 | -13.437 | 1.00 | 0.00 | 3A4 |
| ATOM | 2270 | OE1 | GLN | 331 | 31.063 | 15.988 | -13.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 2271 | NE2 | GLN | 331 | 32.677 | 14.396 | -13.885 | 1.00 | 0.00 | 3A4 |
| ATOM | 2272 | C   | GLN | 331 | 34.500 | 19.817 | -12.447 | 1.00 | 0.00 | 3A4 |
| ATOM | 2273 | O   | GLN | 331 | 35.682 | 19.821 | -12.771 | 1.00 | 0.00 | 3A4 |
| ATOM | 2274 | N   | GLU | 332 | 33.723 | 20.913 | -12.594 | 1.00 | 0.00 | 3A4 |
| ATOM | 2275 | CA  | GLU | 332 | 34.188 | 22.185 | -13.099 | 1.00 | 0.00 | 3A4 |
| ATOM | 2276 | CB  | GLU | 332 | 33.019 | 23.173 | -13.413 | 1.00 | 0.00 | 3A4 |
| ATOM | 2277 | CG  | GLU | 332 | 32.212 | 22.808 | -14.675 | 1.00 | 0.00 | 3A4 |
| ATOM | 2278 | CD  | GLU | 332 | 33.080 | 22.951 | -15.931 | 1.00 | 0.00 | 3A4 |
| ATOM | 2279 | OE1 | GLU | 332 | 33.533 | 24.092 | -16.217 | 1.00 | 0.00 | 3A4 |
| ATOM | 2280 | OE2 | GLU | 332 | 33.301 | 21.919 | -16.622 | 1.00 | 0.00 | 3A4 |
| ATOM | 2281 | C   | GLU | 332 | 35.190 | 22.869 | -12.182 | 1.00 | 0.00 | 3A4 |
| ATOM | 2282 | O   | GLU | 332 | 35.834 | 23.799 | -12.629 | 1.00 | 0.00 | 3A4 |
| ATOM | 2283 | N   | GLU | 333 | 35.484 | 22.350 | -10.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 2284 | CA  | GLU | 333 | 36.662 | 22.661 | -10.132 | 1.00 | 0.00 | 3A4 |
| ATOM | 2285 | CB  | GLU | 333 | 36.449 | 22.284 | -8.639  | 1.00 | 0.00 | 3A4 |
| ATOM | 2286 | CG  | GLU | 333 | 35.228 | 22.936 | -7.985  | 1.00 | 0.00 | 3A4 |
| ATOM | 2287 | CD  | GLU | 333 | 35.046 | 22.273 | -6.620  | 1.00 | 0.00 | 3A4 |
| ATOM | 2288 | OE1 | GLU | 333 | 35.918 | 22.455 | -5.730  | 1.00 | 0.00 | 3A4 |
| ATOM | 2289 | OE2 | GLU | 333 | 34.038 | 21.540 | -6.462  | 1.00 | 0.00 | 3A4 |
| ATOM | 2290 | C   | GLU | 333 | 37.923 | 21.912 | -10.581 | 1.00 | 0.00 | 3A4 |
| ATOM | 2291 | O   | GLU | 333 | 38.425 | 21.038 | -9.874  | 1.00 | 0.00 | 3A4 |
| ATOM | 2292 | N   | ILE | 334 | 38.469 | 22.262 | -11.773 | 1.00 | 0.00 | 3A4 |
| ATOM | 2293 | CA  | ILE | 334 | 39.710 | 21.726 | -12.300 | 1.00 | 0.00 | 3A4 |
| ATOM | 2294 | CB  | ILE | 334 | 39.559 | 20.353 | -12.973 | 1.00 | 0.00 | 3A4 |
| ATOM | 2295 | CG2 | ILE | 334 | 38.582 | 20.368 | -14.182 | 1.00 | 0.00 | 3A4 |
| ATOM | 2296 | CG1 | ILE | 334 | 40.932 | 19.687 | -13.257 | 1.00 | 0.00 | 3A4 |
| ATOM | 2297 | CD  | ILE | 334 | 40.838 | 18.213 | -13.660 | 1.00 | 0.00 | 3A4 |
| ATOM | 2298 | C   | ILE | 334 | 40.231 | 22.836 | -13.189 | 1.00 | 0.00 | 3A4 |
| ATOM | 2299 | O   | ILE | 334 | 40.570 | 22.658 | -14.358 | 1.00 | 0.00 | 3A4 |
| ATOM | 2300 | N   | ASP | 335 | 40.294 | 24.063 | -12.600 | 1.00 | 0.00 | 3A4 |
| ATOM | 2301 | CA  | ASP | 335 | 40.593 | 25.320 | -13.260 | 1.00 | 0.00 | 3A4 |
| ATOM | 2302 | CB  | ASP | 335 | 39.726 | 26.490 | -12.699 | 1.00 | 0.00 | 3A4 |
| ATOM | 2303 | CG  | ASP | 335 | 38.240 | 26.203 | -12.943 | 1.00 | 0.00 | 3A4 |
| ATOM | 2304 | OD1 | ASP | 335 | 37.854 | 26.015 | -14.129 | 1.00 | 0.00 | 3A4 |
| ATOM | 2305 | OD2 | ASP | 335 | 37.469 | 26.175 | -11.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 2306 | C   | ASP | 335 | 42.054 | 25.655 | -13.079 | 1.00 | 0.00 | 3A4 |
| ATOM | 2307 | O   | ASP | 335 | 42.537 | 25.781 | -11.956 | 1.00 | 0.00 | 3A4 |
| ATOM | 2308 | N   | ALA | 336 | 42.772 | 25.816 | -14.223 | 1.00 | 0.00 | 3A4 |
| ATOM | 2309 | CA  | ALA | 336 | 44.168 | 26.192 | -14.316 | 1.00 | 0.00 | 3A4 |
| ATOM | 2310 | CB  | ALA | 336 | 45.027 | 25.116 | -15.028 | 1.00 | 0.00 | 3A4 |
| ATOM | 2311 | C   | ALA | 336 | 44.207 | 27.500 | -15.065 | 1.00 | 0.00 | 3A4 |
| ATOM | 2312 | O   | ALA | 336 | 44.428 | 27.544 | -16.275 | 1.00 | 0.00 | 3A4 |
| ATOM | 2313 | N   | VAL | 337 | 43.963 | 28.609 | -14.313 | 1.00 | 0.00 | 3A4 |
| ATOM | 2314 | CA  | VAL | 337 | 43.815 | 29.978 | -14.773 | 1.00 | 0.00 | 3A4 |
| ATOM | 2315 | CB  | VAL | 337 | 42.641 | 30.686 | -14.085 | 1.00 | 0.00 | 3A4 |
| ATOM | 2316 | CG1 | VAL | 337 | 42.436 | 32.130 | -14.612 | 1.00 | 0.00 | 3A4 |
| ATOM | 2317 | CG2 | VAL | 337 | 41.367 | 29.847 | -14.326 | 1.00 | 0.00 | 3A4 |
| ATOM | 2318 | C   | VAL | 337 | 45.115 | 30.696 | -14.492 | 1.00 | 0.00 | 3A4 |
| ATOM | 2319 | O   | VAL | 337 | 45.661 | 30.605 | -13.394 | 1.00 | 0.00 | 3A4 |
| ATOM | 2320 | N   | LEU | 338 | 45.621 | 31.439 | -15.517 | 1.00 | 0.00 | 3A4 |
| ATOM | 2321 | CA  | LEU | 338 | 46.821 | 32.257 | -15.500 | 1.00 | 0.00 | 3A4 |
| ATOM | 2322 | CB  | LEU | 338 | 47.678 | 32.088 | -16.799 | 1.00 | 0.00 | 3A4 |
| ATOM | 2323 | CG  | LEU | 338 | 48.507 | 30.778 | -16.897 | 1.00 | 0.00 | 3A4 |
| ATOM | 2324 | CD1 | LEU | 338 | 47.680 | 29.494 | -17.124 | 1.00 | 0.00 | 3A4 |
| ATOM | 2325 | CD2 | LEU | 338 | 49.592 | 30.909 | -17.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 2326 | C   | LEU | 338 | 46.355 | 33.705 | -15.361 | 1.00 | 0.00 | 3A4 |
| ATOM | 2327 | O   | LEU | 338 | 45.265 | 34.009 | -15.844 | 1.00 | 0.00 | 3A4 |
| ATOM | 2328 | N   | PRO | 339 | 47.103 | 34.638 | -14.719 | 1.00 | 0.00 | 3A4 |
| ATOM | 2329 | CA  | PRO | 339 | 46.612 | 35.949 | -14.286 | 1.00 | 0.00 | 3A4 |
| ATOM | 2330 | CD  | PRO | 339 | 48.443 | 34.363 | -14.196 | 1.00 | 0.00 | 3A4 |
| ATOM | 2331 | CB  | PRO | 339 | 47.610 | 36.376 | -13.189 | 1.00 | 0.00 | 3A4 |
| ATOM | 2332 | CG  | PRO | 339 | 48.922 | 35.669 | -13.552 | 1.00 | 0.00 | 3A4 |
| ATOM | 2333 | C   | PRO | 339 | 46.561 | 36.955 | -15.437 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 2334 | O   | PRO | 339 | 47.465 | 36.980 | -16.272 | 1.00 | 0.00 | 3A4 |
| ATOM | 2335 | N   | ASN | 340 | 45.491 | 37.790 | -15.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 2336 | CA  | ASN | 340 | 45.246 | 38.810 | -16.464 | 1.00 | 0.00 | 3A4 |
| ATOM | 2337 | CB  | ASN | 340 | 44.189 | 38.343 | -17.523 | 1.00 | 0.00 | 3A4 |
| ATOM | 2338 | CG  | ASN | 340 | 44.036 | 39.320 | -18.704 | 1.00 | 0.00 | 3A4 |
| ATOM | 2339 | OD1 | ASN | 340 | 42.986 | 39.942 | -18.858 | 1.00 | 0.00 | 3A4 |
| ATOM | 2340 | ND2 | ASN | 340 | 45.094 | 39.457 | -19.550 | 1.00 | 0.00 | 3A4 |
| ATOM | 2341 | C   | ASN | 340 | 44.785 | 40.012 | -15.672 | 1.00 | 0.00 | 3A4 |
| ATOM | 2342 | O   | ASN | 340 | 45.452 | 41.045 | -15.645 | 1.00 | 0.00 | 3A4 |
| ATOM | 2343 | N   | LYS | 341 | 43.617 | 39.870 | -14.997 | 1.00 | 0.00 | 3A4 |
| ATOM | 2344 | CA  | LYS | 341 | 43.059 | 40.852 | -14.095 | 1.00 | 0.00 | 3A4 |
| ATOM | 2345 | CB  | LYS | 341 | 42.250 | 41.970 | -14.822 | 1.00 | 0.00 | 3A4 |
| ATOM | 2346 | CG  | LYS | 341 | 41.892 | 43.181 | -13.936 | 1.00 | 0.00 | 3A4 |
| ATOM | 2347 | CD  | LYS | 341 | 41.220 | 44.359 | -14.664 | 1.00 | 0.00 | 3A4 |
| ATOM | 2348 | CE  | LYS | 341 | 39.708 | 44.212 | -14.924 | 1.00 | 0.00 | 3A4 |
| ATOM | 2349 | NZ  | LYS | 341 | 39.409 | 43.231 | -15.994 | 1.00 | 0.00 | 3A4 |
| ATOM | 2350 | C   | LYS | 341 | 42.197 | 40.042 | -13.158 | 1.00 | 0.00 | 3A4 |
| ATOM | 2351 | O   | LYS | 341 | 40.991 | 40.258 | -13.036 | 1.00 | 0.00 | 3A4 |
| ATOM | 2352 | N   | ALA | 342 | 42.834 | 39.053 | -12.482 | 1.00 | 0.00 | 3A4 |
| ATOM | 2353 | CA  | ALA | 342 | 42.189 | 38.131 | -11.577 | 1.00 | 0.00 | 3A4 |
| ATOM | 2354 | CB  | ALA | 342 | 41.316 | 37.064 | -12.306 | 1.00 | 0.00 | 3A4 |
| ATOM | 2355 | C   | ALA | 342 | 43.313 | 37.430 | -10.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 2356 | O   | ALA | 342 | 44.413 | 37.344 | -11.386 | 1.00 | 0.00 | 3A4 |
| ATOM | 2357 | N   | PRO | 343 | 43.106 | 36.880 | -9.614  | 1.00 | 0.00 | 3A4 |
| ATOM | 2358 | CA  | PRO | 343 | 44.072 | 36.050 | -8.891  | 1.00 | 0.00 | 3A4 |
| ATOM | 2359 | CD  | PRO | 343 | 41.953 | 37.220 | -8.779  | 1.00 | 0.00 | 3A4 |
| ATOM | 2360 | CB  | PRO | 343 | 43.605 | 36.121 | -7.421  | 1.00 | 0.00 | 3A4 |
| ATOM | 2361 | CG  | PRO | 343 | 42.097 | 36.392 | -7.496  | 1.00 | 0.00 | 3A4 |
| ATOM | 2362 | C   | PRO | 343 | 44.071 | 34.607 | -9.441  | 1.00 | 0.00 | 3A4 |
| ATOM | 2363 | O   | PRO | 343 | 42.970 | 34.083 | -9.619  | 1.00 | 0.00 | 3A4 |
| ATOM | 2364 | N   | PRO | 344 | 45.209 | 33.930 | -9.727  | 1.00 | 0.00 | 3A4 |
| ATOM | 2365 | CA  | PRO | 344 | 45.259 | 32.659 | -10.448 | 1.00 | 0.00 | 3A4 |
| ATOM | 2366 | CD  | PRO | 344 | 46.542 | 34.509 | -9.559  | 1.00 | 0.00 | 3A4 |
| ATOM | 2367 | CB  | PRO | 344 | 46.678 | 32.636 | -11.047 | 1.00 | 0.00 | 3A4 |
| ATOM | 2368 | CG  | PRO | 344 | 47.532 | 33.459 | -10.077 | 1.00 | 0.00 | 3A4 |
| ATOM | 2369 | C   | PRO | 344 | 45.002 | 31.473 | -9.520  | 1.00 | 0.00 | 3A4 |
| ATOM | 2370 | O   | PRO | 344 | 45.522 | 31.443 | -8.404  | 1.00 | 0.00 | 3A4 |
| ATOM | 2371 | N   | THR | 345 | 44.206 | 30.483 | -10.004 | 1.00 | 0.00 | 3A4 |
| ATOM | 2372 | CA  | THR | 345 | 43.860 | 29.247 | -9.324  | 1.00 | 0.00 | 3A4 |
| ATOM | 2373 | CB  | THR | 345 | 42.343 | 29.124 | -9.107  | 1.00 | 0.00 | 3A4 |
| ATOM | 2374 | OG1 | THR | 345 | 41.981 | 27.994 | -8.315  | 1.00 | 0.00 | 3A4 |
| ATOM | 2375 | CG2 | THR | 345 | 41.532 | 29.140 | -10.430 | 1.00 | 0.00 | 3A4 |
| ATOM | 2376 | C   | THR | 345 | 44.457 | 28.142 | -10.173 | 1.00 | 0.00 | 3A4 |
| ATOM | 2377 | O   | THR | 345 | 44.489 | 28.242 | -11.397 | 1.00 | 0.00 | 3A4 |
| ATOM | 2378 | N   | TYR | 346 | 44.964 | 27.063 | -9.521  | 1.00 | 0.00 | 3A4 |
| ATOM | 2379 | CA  | TYR | 346 | 45.601 | 25.934 | -10.173 | 1.00 | 0.00 | 3A4 |
| ATOM | 2380 | CB  | TYR | 346 | 47.162 | 25.970 | -10.121 | 1.00 | 0.00 | 3A4 |
| ATOM | 2381 | CG  | TYR | 346 | 47.679 | 27.135 | -10.925 | 1.00 | 0.00 | 3A4 |
| ATOM | 2382 | CD1 | TYR | 346 | 48.250 | 28.252 | -10.287 | 1.00 | 0.00 | 3A4 |
| ATOM | 2383 | CD2 | TYR | 346 | 47.581 | 27.136 | -12.331 | 1.00 | 0.00 | 3A4 |
| ATOM | 2384 | CE1 | TYR | 346 | 48.713 | 29.345 | -11.032 | 1.00 | 0.00 | 3A4 |
| ATOM | 2385 | CE2 | TYR | 346 | 48.037 | 28.229 | -13.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 2386 | CZ  | TYR | 346 | 48.606 | 29.335 | -12.431 | 1.00 | 0.00 | 3A4 |
| ATOM | 2387 | OH  | TYR | 346 | 49.065 | 30.442 | -13.178 | 1.00 | 0.00 | 3A4 |
| ATOM | 2388 | C   | TYR | 346 | 45.106 | 24.709 | -9.453  | 1.00 | 0.00 | 3A4 |
| ATOM | 2389 | O   | TYR | 346 | 45.423 | 24.491 | -8.285  | 1.00 | 0.00 | 3A4 |
| ATOM | 2390 | N   | ASP | 347 | 44.302 | 23.879 | -10.168 | 1.00 | 0.00 | 3A4 |
| ATOM | 2391 | CA  | ASP | 347 | 43.715 | 22.647 | -9.683  | 1.00 | 0.00 | 3A4 |
| ATOM | 2392 | CB  | ASP | 347 | 42.187 | 22.761 | -9.384  | 1.00 | 0.00 | 3A4 |
| ATOM | 2393 | CG  | ASP | 347 | 41.948 | 23.760 | -8.248  | 1.00 | 0.00 | 3A4 |
| ATOM | 2394 | OD1 | ASP | 347 | 41.329 | 24.825 | -8.516  | 1.00 | 0.00 | 3A4 |
| ATOM | 2395 | OD2 | ASP | 347 | 42.386 | 23.474 | -7.102  | 1.00 | 0.00 | 3A4 |
| ATOM | 2396 | C   | ASP | 347 | 43.937 | 21.639 | -10.781 | 1.00 | 0.00 | 3A4 |
| ATOM | 2397 | O   | ASP | 347 | 43.549 | 21.862 | -11.927 | 1.00 | 0.00 | 3A4 |
| ATOM | 2398 | N   | THR | 348 | 44.581 | 20.493 | -10.427 | 1.00 | 0.00 | 3A4 |
| ATOM | 2399 | CA  | THR | 348 | 44.908 | 19.388 | -11.314 | 1.00 | 0.00 | 3A4 |
| ATOM | 2400 | CB  | THR | 348 | 46.416 | 19.199 | -11.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 2401 | OG1 | THR | 348 | 46.987 | 20.401 | -12.006 | 1.00 | 0.00 | 3A4 |
| ATOM | 2402 | CG2 | THR | 348 | 46.725 | 18.051 | -12.500 | 1.00 | 0.00 | 3A4 |
| ATOM | 2403 | C   | THR | 348 | 44.258 | 18.178 | -10.688 | 1.00 | 0.00 | 3A4 |
| ATOM | 2404 | O   | THR | 348 | 43.393 | 17.548 | -11.293 | 1.00 | 0.00 | 3A4 |
| ATOM | 2405 | N   | VAL | 349 | 44.670 | 17.854 | -9.434  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2406 | CA  | VAL | 349 | 44.059 | 16.848 | -8.590 | 1.00 | 0.00 | 3A4 |
| ATOM | 2407 | CB  | VAL | 349 | 44.630 | 15.437 | -8.788 | 1.00 | 0.00 | 3A4 |
| ATOM | 2408 | CG1 | VAL | 349 | 46.169 | 15.347 | -8.617 | 1.00 | 0.00 | 3A4 |
| ATOM | 2409 | CG2 | VAL | 349 | 43.834 | 14.402 | -7.958 | 1.00 | 0.00 | 3A4 |
| ATOM | 2410 | C   | VAL | 349 | 44.175 | 17.435 | -7.201 | 1.00 | 0.00 | 3A4 |
| ATOM | 2411 | O   | VAL | 349 | 44.934 | 16.990 | -6.341 | 1.00 | 0.00 | 3A4 |
| ATOM | 2412 | N   | LEU | 350 | 43.387 | 18.518 | -6.988 | 1.00 | 0.00 | 3A4 |
| ATOM | 2413 | CA  | LEU | 350 | 43.440 | 19.369 | -5.824 | 1.00 | 0.00 | 3A4 |
| ATOM | 2414 | CB  | LEU | 350 | 44.479 | 20.520 | -6.024 | 1.00 | 0.00 | 3A4 |
| ATOM | 2415 | CG  | LEU | 350 | 44.847 | 21.374 | -4.785 | 1.00 | 0.00 | 3A4 |
| ATOM | 2416 | CD1 | LEU | 350 | 45.497 | 20.539 | -3.662 | 1.00 | 0.00 | 3A4 |
| ATOM | 2417 | CD2 | LEU | 350 | 45.743 | 22.560 | -5.187 | 1.00 | 0.00 | 3A4 |
| ATOM | 2418 | C   | LEU | 350 | 42.042 | 19.913 | -5.672 | 1.00 | 0.00 | 3A4 |
| ATOM | 2419 | O   | LEU | 350 | 41.270 | 19.945 | -6.631 | 1.00 | 0.00 | 3A4 |
| ATOM | 2420 | N   | GLN | 351 | 41.689 | 20.372 | -4.436 | 1.00 | 0.00 | 3A4 |
| ATOM | 2421 | CA  | GLN | 351 | 40.404 | 20.942 | -4.059 | 1.00 | 0.00 | 3A4 |
| ATOM | 2422 | CB  | GLN | 351 | 40.005 | 20.645 | -2.573 | 1.00 | 0.00 | 3A4 |
| ATOM | 2423 | CG  | GLN | 351 | 40.814 | 21.289 | -1.417 | 1.00 | 0.00 | 3A4 |
| ATOM | 2424 | CD  | GLN | 351 | 42.269 | 20.816 | -1.386 | 1.00 | 0.00 | 3A4 |
| ATOM | 2425 | OE1 | GLN | 351 | 43.177 | 21.634 | -1.520 | 1.00 | 0.00 | 3A4 |
| ATOM | 2426 | NE2 | GLN | 351 | 42.505 | 19.487 | -1.200 | 1.00 | 0.00 | 3A4 |
| ATOM | 2427 | C   | GLN | 351 | 40.390 | 22.432 | -4.305 | 1.00 | 0.00 | 3A4 |
| ATOM | 2428 | O   | GLN | 351 | 41.399 | 23.112 | -4.117 | 1.00 | 0.00 | 3A4 |
| ATOM | 2429 | N   | MET | 352 | 39.214 | 22.962 | -4.740 | 1.00 | 0.00 | 3A4 |
| ATOM | 2430 | CA  | MET | 352 | 38.994 | 24.368 | -5.014 | 1.00 | 0.00 | 3A4 |
| ATOM | 2431 | CB  | MET | 352 | 38.436 | 24.632 | -6.438 | 1.00 | 0.00 | 3A4 |
| ATOM | 2432 | CG  | MET | 352 | 38.472 | 26.097 | -6.900 | 1.00 | 0.00 | 3A4 |
| ATOM | 2433 | SD  | MET | 352 | 37.969 | 26.316 | -8.633 | 1.00 | 0.00 | 3A4 |
| ATOM | 2434 | CE  | MET | 352 | 38.075 | 28.129 | -8.608 | 1.00 | 0.00 | 3A4 |
| ATOM | 2435 | C   | MET | 352 | 38.113 | 24.911 | -3.914 | 1.00 | 0.00 | 3A4 |
| ATOM | 2436 | O   | MET | 352 | 38.636 | 25.287 | -2.866 | 1.00 | 0.00 | 3A4 |
| ATOM | 2437 | N   | GLU | 353 | 36.765 | 25.000 | -4.117 | 1.00 | 0.00 | 3A4 |
| ATOM | 2438 | CA  | GLU | 353 | 35.914 | 25.749 | -3.211 | 1.00 | 0.00 | 3A4 |
| ATOM | 2439 | CB  | GLU | 353 | 35.689 | 27.217 | -3.688 | 1.00 | 0.00 | 3A4 |
| ATOM | 2440 | CG  | GLU | 353 | 36.922 | 28.142 | -3.627 | 1.00 | 0.00 | 3A4 |
| ATOM | 2441 | CD  | GLU | 353 | 36.543 | 29.540 | -4.126 | 1.00 | 0.00 | 3A4 |
| ATOM | 2442 | OE1 | GLU | 353 | 36.622 | 30.504 | -3.318 | 1.00 | 0.00 | 3A4 |
| ATOM | 2443 | OE2 | GLU | 353 | 36.171 | 29.660 | -5.325 | 1.00 | 0.00 | 3A4 |
| ATOM | 2444 | C   | GLU | 353 | 34.592 | 25.102 | -2.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 2445 | O   | GLU | 353 | 34.078 | 25.104 | -1.864 | 1.00 | 0.00 | 3A4 |
| ATOM | 2446 | N   | TYR | 354 | 33.979 | 24.537 | -4.047 | 1.00 | 0.00 | 3A4 |
| ATOM | 2447 | CA  | TYR | 354 | 32.629 | 24.016 | -3.996 | 1.00 | 0.00 | 3A4 |
| ATOM | 2448 | CB  | TYR | 354 | 31.928 | 24.005 | -5.369 | 1.00 | 0.00 | 3A4 |
| ATOM | 2449 | CG  | TYR | 354 | 31.880 | 25.395 | -5.954 | 1.00 | 0.00 | 3A4 |
| ATOM | 2450 | CD1 | TYR | 354 | 32.962 | 25.916 | -6.691 | 1.00 | 0.00 | 3A4 |
| ATOM | 2451 | CD2 | TYR | 354 | 30.740 | 26.199 | -5.783 | 1.00 | 0.00 | 3A4 |
| ATOM | 2452 | CE1 | TYR | 354 | 32.917 | 27.212 | -7.224 | 1.00 | 0.00 | 3A4 |
| ATOM | 2453 | CE2 | TYR | 354 | 30.683 | 27.496 | -6.314 | 1.00 | 0.00 | 3A4 |
| ATOM | 2454 | CZ  | TYR | 354 | 31.774 | 28.004 | -7.035 | 1.00 | 0.00 | 3A4 |
| ATOM | 2455 | OH  | TYR | 354 | 31.722 | 29.310 | -7.571 | 1.00 | 0.00 | 3A4 |
| ATOM | 2456 | C   | TYR | 354 | 32.592 | 22.628 | -3.428 | 1.00 | 0.00 | 3A4 |
| ATOM | 2457 | O   | TYR | 354 | 31.575 | 22.220 | -2.892 | 1.00 | 0.00 | 3A4 |
| ATOM | 2458 | N   | LEU | 355 | 33.710 | 21.867 | -3.466 | 1.00 | 0.00 | 3A4 |
| ATOM | 2459 | CA  | LEU | 355 | 33.715 | 20.493 | -2.996 | 1.00 | 0.00 | 3A4 |
| ATOM | 2460 | CB  | LEU | 355 | 34.970 | 19.771 | -3.512 | 1.00 | 0.00 | 3A4 |
| ATOM | 2461 | CG  | LEU | 355 | 34.521 | 18.784 | -4.631 | 1.00 | 0.00 | 3A4 |
| ATOM | 2462 | CD1 | LEU | 355 | 35.547 | 18.525 | -5.749 | 1.00 | 0.00 | 3A4 |
| ATOM | 2463 | CD2 | LEU | 355 | 33.945 | 17.479 | -4.064 | 1.00 | 0.00 | 3A4 |
| ATOM | 2464 | C   | LEU | 355 | 33.573 | 20.380 | -1.485 | 1.00 | 0.00 | 3A4 |
| ATOM | 2465 | O   | LEU | 355 | 32.806 | 19.570 | -0.980 | 1.00 | 0.00 | 3A4 |
| ATOM | 2466 | N   | ASP | 356 | 34.225 | 21.283 | -0.721 | 1.00 | 0.00 | 3A4 |
| ATOM | 2467 | CA  | ASP | 356 | 34.070 | 21.466 | 0.714  | 1.00 | 0.00 | 3A4 |
| ATOM | 2468 | CB  | ASP | 356 | 34.921 | 22.723 | 1.144  | 1.00 | 0.00 | 3A4 |
| ATOM | 2469 | CG  | ASP | 356 | 35.819 | 22.461 | 2.358  | 1.00 | 0.00 | 3A4 |
| ATOM | 2470 | OD1 | ASP | 356 | 35.262 | 22.182 | 3.454  | 1.00 | 0.00 | 3A4 |
| ATOM | 2471 | OD2 | ASP | 356 | 37.067 | 22.560 | 2.214  | 1.00 | 0.00 | 3A4 |
| ATOM | 2472 | C   | ASP | 356 | 32.651 | 21.700 | 1.182  | 1.00 | 0.00 | 3A4 |
| ATOM | 2473 | O   | ASP | 356 | 32.180 | 21.110 | 2.149  | 1.00 | 0.00 | 3A4 |
| ATOM | 2474 | N   | MET | 357 | 31.928 | 22.551 | 0.423  | 1.00 | 0.00 | 3A4 |
| ATOM | 2475 | CA  | MET | 357 | 30.540 | 22.879 | 0.616  | 1.00 | 0.00 | 3A4 |
| ATOM | 2476 | CB  | MET | 357 | 30.168 | 24.100 | -0.239 | 1.00 | 0.00 | 3A4 |
| ATOM | 2477 | CG  | MET | 357 | 29.601 | 25.250 | 0.627  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2478 | SD  | MET | 357 | 30.612 | 26.763 | 0.665  | 1.00 | 0.00 | 3A4 |
| ATOM | 2479 | CE  | MET | 357 | 29.381 | 27.754 | 1.562  | 1.00 | 0.00 | 3A4 |
| ATOM | 2480 | C   | MET | 357 | 29.622 | 21.737 | 0.289  | 1.00 | 0.00 | 3A4 |
| ATOM | 2481 | O   | MET | 357 | 28.618 | 21.519 | 0.952  | 1.00 | 0.00 | 3A4 |
| ATOM | 2482 | N   | VAL | 358 | 29.995 | 20.909 | -0.714 | 1.00 | 0.00 | 3A4 |
| ATOM | 2483 | CA  | VAL | 358 | 29.302 | 19.693 | -1.096 | 1.00 | 0.00 | 3A4 |
| ATOM | 2484 | CB  | VAL | 358 | 29.848 | 19.071 | -2.374 | 1.00 | 0.00 | 3A4 |
| ATOM | 2485 | CG1 | VAL | 358 | 29.224 | 17.667 | -2.681 | 1.00 | 0.00 | 3A4 |
| ATOM | 2486 | CG2 | VAL | 358 | 29.530 | 20.074 | -3.459 | 1.00 | 0.00 | 3A4 |
| ATOM | 2487 | C   | VAL | 358 | 29.376 | 18.671 | 0.012  | 1.00 | 0.00 | 3A4 |
| ATOM | 2488 | O   | VAL | 358 | 28.364 | 18.076 | 0.363  | 1.00 | 0.00 | 3A4 |
| ATOM | 2489 | N   | VAL | 359 | 30.567 | 18.479 | 0.633  | 1.00 | 0.00 | 3A4 |
| ATOM | 2490 | CA  | VAL | 359 | 30.783 | 17.579 | 1.758  | 1.00 | 0.00 | 3A4 |
| ATOM | 2491 | CB  | VAL | 359 | 32.264 | 17.531 | 2.146  | 1.00 | 0.00 | 3A4 |
| ATOM | 2492 | CG1 | VAL | 359 | 32.553 | 16.768 | 3.459  | 1.00 | 0.00 | 3A4 |
| ATOM | 2493 | CG2 | VAL | 359 | 33.043 | 16.854 | 1.004  | 1.00 | 0.00 | 3A4 |
| ATOM | 2494 | C   | VAL | 359 | 29.954 | 17.977 | 2.962  | 1.00 | 0.00 | 3A4 |
| ATOM | 2495 | O   | VAL | 359 | 29.303 | 17.151 | 3.591  | 1.00 | 0.00 | 3A4 |
| ATOM | 2496 | N   | ASN | 360 | 29.903 | 19.287 | 3.263  | 1.00 | 0.00 | 3A4 |
| ATOM | 2497 | CA  | ASN | 360 | 29.117 | 19.830 | 4.350  | 1.00 | 0.00 | 3A4 |
| ATOM | 2498 | CB  | ASN | 360 | 29.412 | 21.328 | 4.537  | 1.00 | 0.00 | 3A4 |
| ATOM | 2499 | CG  | ASN | 360 | 30.795 | 21.548 | 5.189  | 1.00 | 0.00 | 3A4 |
| ATOM | 2500 | OD1 | ASN | 360 | 31.725 | 20.750 | 5.080  | 1.00 | 0.00 | 3A4 |
| ATOM | 2501 | ND2 | ASN | 360 | 30.946 | 22.706 | 5.890  | 1.00 | 0.00 | 3A4 |
| ATOM | 2502 | C   | ASN | 360 | 27.624 | 19.645 | 4.147  | 1.00 | 0.00 | 3A4 |
| ATOM | 2503 | O   | ASN | 360 | 26.891 | 19.274 | 5.060  | 1.00 | 0.00 | 3A4 |
| ATOM | 2504 | N   | GLU | 361 | 27.149 | 19.820 | 2.890  | 1.00 | 0.00 | 3A4 |
| ATOM | 2505 | CA  | GLU | 361 | 25.768 | 19.606 | 2.527  | 1.00 | 0.00 | 3A4 |
| ATOM | 2506 | CB  | GLU | 361 | 25.458 | 20.211 | 1.139  | 1.00 | 0.00 | 3A4 |
| ATOM | 2507 | CG  | GLU | 361 | 24.026 | 19.998 | 0.629  | 1.00 | 0.00 | 3A4 |
| ATOM | 2508 | CD  | GLU | 361 | 22.935 | 20.638 | 1.489  | 1.00 | 0.00 | 3A4 |
| ATOM | 2509 | OE1 | GLU | 361 | 23.253 | 21.306 | 2.504  | 1.00 | 0.00 | 3A4 |
| ATOM | 2510 | OE2 | GLU | 361 | 21.740 | 20.442 | 1.143  | 1.00 | 0.00 | 3A4 |
| ATOM | 2511 | C   | GLU | 361 | 25.372 | 18.147 | 2.553  | 1.00 | 0.00 | 3A4 |
| ATOM | 2512 | O   | GLU | 361 | 24.258 | 17.809 | 2.941  | 1.00 | 0.00 | 3A4 |
| ATOM | 2513 | N   | THR | 362 | 26.285 | 17.210 | 2.205  | 1.00 | 0.00 | 3A4 |
| ATOM | 2514 | CA  | THR | 362 | 26.034 | 15.779 | 2.269  | 1.00 | 0.00 | 3A4 |
| ATOM | 2515 | CB  | THR | 362 | 27.109 | 14.973 | 1.573  | 1.00 | 0.00 | 3A4 |
| ATOM | 2516 | OG1 | THR | 362 | 27.154 | 15.360 | 0.208  | 1.00 | 0.00 | 3A4 |
| ATOM | 2517 | CG2 | THR | 362 | 26.766 | 13.462 | 1.673  | 1.00 | 0.00 | 3A4 |
| ATOM | 2518 | C   | THR | 362 | 25.886 | 15.303 | 3.702  | 1.00 | 0.00 | 3A4 |
| ATOM | 2519 | O   | THR | 362 | 24.990 | 14.527 | 4.020  | 1.00 | 0.00 | 3A4 |
| ATOM | 2520 | N   | LEU | 363 | 26.722 | 15.835 | 4.611  | 1.00 | 0.00 | 3A4 |
| ATOM | 2521 | CA  | LEU | 363 | 26.677 | 15.555 | 6.026  | 1.00 | 0.00 | 3A4 |
| ATOM | 2522 | CB  | LEU | 363 | 27.934 | 16.102 | 6.729  | 1.00 | 0.00 | 3A4 |
| ATOM | 2523 | CG  | LEU | 363 | 29.216 | 15.310 | 6.428  | 1.00 | 0.00 | 3A4 |
| ATOM | 2524 | CD1 | LEU | 363 | 30.434 | 16.188 | 6.740  | 1.00 | 0.00 | 3A4 |
| ATOM | 2525 | CD2 | LEU | 363 | 29.238 | 13.981 | 7.211  | 1.00 | 0.00 | 3A4 |
| ATOM | 2526 | C   | LEU | 363 | 25.448 | 16.157 | 6.698  | 1.00 | 0.00 | 3A4 |
| ATOM | 2527 | O   | LEU | 363 | 24.956 | 15.614 | 7.681  | 1.00 | 0.00 | 3A4 |
| ATOM | 2528 | N   | ARG | 364 | 24.890 | 17.274 | 6.163  | 1.00 | 0.00 | 3A4 |
| ATOM | 2529 | CA  | ARG | 364 | 23.659 | 17.879 | 6.633  | 1.00 | 0.00 | 3A4 |
| ATOM | 2530 | CB  | ARG | 364 | 23.446 | 19.303 | 6.082  | 1.00 | 0.00 | 3A4 |
| ATOM | 2531 | CG  | ARG | 364 | 22.238 | 20.031 | 6.676  | 1.00 | 0.00 | 3A4 |
| ATOM | 2532 | CD  | ARG | 364 | 22.212 | 21.544 | 6.417  | 1.00 | 0.00 | 3A4 |
| ATOM | 2533 | NE  | ARG | 364 | 21.256 | 22.182 | 7.393  | 1.00 | 0.00 | 3A4 |
| ATOM | 2534 | CZ  | ARG | 364 | 21.624 | 22.741 | 8.595  | 1.00 | 0.00 | 3A4 |
| ATOM | 2535 | NH1 | ARG | 364 | 20.663 | 23.251 | 9.418  | 1.00 | 0.00 | 3A4 |
| ATOM | 2536 | NH2 | ARG | 364 | 22.925 | 22.809 | 8.992  | 1.00 | 0.00 | 3A4 |
| ATOM | 2537 | C   | ARG | 364 | 22.463 | 17.060 | 6.233  | 1.00 | 0.00 | 3A4 |
| ATOM | 2538 | O   | ARG | 364 | 21.622 | 16.711 | 7.049  | 1.00 | 0.00 | 3A4 |
| ATOM | 2539 | N   | LEU | 365 | 22.393 | 16.685 | 4.940  | 1.00 | 0.00 | 3A4 |
| ATOM | 2540 | CA  | LEU | 365 | 21.267 | 15.979 | 4.384  | 1.00 | 0.00 | 3A4 |
| ATOM | 2541 | CB  | LEU | 365 | 21.247 | 16.050 | 2.848  | 1.00 | 0.00 | 3A4 |
| ATOM | 2542 | CG  | LEU | 365 | 19.879 | 16.592 | 2.326  | 1.00 | 0.00 | 3A4 |
| ATOM | 2543 | CD1 | LEU | 365 | 19.837 | 16.585 | 0.811  | 1.00 | 0.00 | 3A4 |
| ATOM | 2544 | CD2 | LEU | 365 | 18.607 | 15.874 | 2.828  | 1.00 | 0.00 | 3A4 |
| ATOM | 2545 | C   | LEU | 365 | 21.135 | 14.540 | 4.810  | 1.00 | 0.00 | 3A4 |
| ATOM | 2546 | O   | LEU | 365 | 20.029 | 14.082 | 5.089  | 1.00 | 0.00 | 3A4 |
| ATOM | 2547 | N   | PHE | 366 | 22.252 | 13.787 | 4.904  | 1.00 | 0.00 | 3A4 |
| ATOM | 2548 | CA  | PHE | 366 | 22.226 | 12.409 | 5.376  | 1.00 | 0.00 | 3A4 |
| ATOM | 2549 | CB  | PHE | 366 | 22.642 | 11.385 | 4.273  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2550 | CG  | PHE | 366 | 21.503 | 11.244 | 3.297  | 1.00 | 0.00 | 3A4 |
| ATOM | 2551 | CD1 | PHE | 366 | 21.538 | 11.861 | 2.035  | 1.00 | 0.00 | 3A4 |
| ATOM | 2552 | CD2 | PHE | 366 | 20.363 | 10.498 | 3.651  | 1.00 | 0.00 | 3A4 |
| ATOM | 2553 | CE1 | PHE | 366 | 20.455 | 11.742 | 1.150  | 1.00 | 0.00 | 3A4 |
| ATOM | 2554 | CE2 | PHE | 366 | 19.278 | 10.377 | 2.773  | 1.00 | 0.00 | 3A4 |
| ATOM | 2555 | CZ  | PHE | 366 | 19.325 | 11.000 | 1.520  | 1.00 | 0.00 | 3A4 |
| ATOM | 2556 | C   | PHE | 366 | 23.116 | 12.273 | 6.585  | 1.00 | 0.00 | 3A4 |
| ATOM | 2557 | O   | PHE | 366 | 24.165 | 11.637 | 6.497  | 1.00 | 0.00 | 3A4 |
| ATOM | 2558 | N   | PRO | 367 | 22.732 | 12.795 | 7.772  | 1.00 | 0.00 | 3A4 |
| ATOM | 2559 | CA  | PRO | 367 | 23.466 | 12.674 | 9.011  | 1.00 | 0.00 | 3A4 |
| ATOM | 2560 | CD  | PRO | 367 | 21.498 | 13.517 | 7.993  | 1.00 | 0.00 | 3A4 |
| ATOM | 2561 | CB  | PRO | 367 | 22.894 | 13.739 | 9.935  | 1.00 | 0.00 | 3A4 |
| ATOM | 2562 | CG  | PRO | 367 | 21.461 | 13.878 | 9.463  | 1.00 | 0.00 | 3A4 |
| ATOM | 2563 | C   | PRO | 367 | 23.332 | 11.269 | 9.536  | 1.00 | 0.00 | 3A4 |
| ATOM | 2564 | O   | PRO | 367 | 22.246 | 10.779 | 9.824  | 1.00 | 0.00 | 3A4 |
| ATOM | 2565 | N   | ILE | 368 | 24.476 | 10.572 | 9.569  | 1.00 | 0.00 | 3A4 |
| ATOM | 2566 | CA  | ILE | 368 | 24.602 | 9.143  | 9.718  | 1.00 | 0.00 | 3A4 |
| ATOM | 2567 | CB  | ILE | 368 | 25.992 | 8.818  | 9.131  | 1.00 | 0.00 | 3A4 |
| ATOM | 2568 | CG2 | ILE | 368 | 27.160 | 9.306  | 10.024 | 1.00 | 0.00 | 3A4 |
| ATOM | 2569 | CG1 | ILE | 368 | 26.230 | 7.413  | 8.553  | 1.00 | 0.00 | 3A4 |
| ATOM | 2570 | CD  | ILE | 368 | 26.421 | 6.268  | 9.546  | 1.00 | 0.00 | 3A4 |
| ATOM | 2571 | C   | ILE | 368 | 24.406 | 8.654  | 11.153 | 1.00 | 0.00 | 3A4 |
| ATOM | 2572 | O   | ILE | 368 | 24.024 | 7.515  | 11.392 | 1.00 | 0.00 | 3A4 |
| ATOM | 2573 | N   | ALA | 369 | 24.661 | 9.530  | 12.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 2574 | CA  | ALA | 369 | 24.719 | 9.183  | 13.542 | 1.00 | 0.00 | 3A4 |
| ATOM | 2575 | CB  | ALA | 369 | 26.067 | 9.640  | 14.141 | 1.00 | 0.00 | 3A4 |
| ATOM | 2576 | C   | ALA | 369 | 23.654 | 9.859  | 14.360 | 1.00 | 0.00 | 3A4 |
| ATOM | 2577 | O   | ALA | 369 | 23.267 | 10.991 | 14.104 | 1.00 | 0.00 | 3A4 |
| ATOM | 2578 | N   | MET | 370 | 23.265 | 9.221  | 15.511 | 1.00 | 0.00 | 3A4 |
| ATOM | 2579 | CA  | MET | 370 | 22.422 | 9.803  | 16.560 | 1.00 | 0.00 | 3A4 |
| ATOM | 2580 | CB  | MET | 370 | 20.964 | 9.264  | 16.470 | 1.00 | 0.00 | 3A4 |
| ATOM | 2581 | CG  | MET | 370 | 19.910 | 10.113 | 17.209 | 1.00 | 0.00 | 3A4 |
| ATOM | 2582 | SD  | MET | 370 | 18.173 | 9.663  | 16.885 | 1.00 | 0.00 | 3A4 |
| ATOM | 2583 | CE  | MET | 370 | 18.081 | 10.195 | 15.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 2584 | C   | MET | 370 | 23.062 | 9.512  | 17.921 | 1.00 | 0.00 | 3A4 |
| ATOM | 2585 | O   | MET | 370 | 23.884 | 8.603  | 18.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 2586 | N   | ARG | 371 | 22.711 | 10.299 | 18.992 | 1.00 | 0.00 | 3A4 |
| ATOM | 2587 | CA  | ARG | 371 | 23.356 | 10.277 | 20.307 | 1.00 | 0.00 | 3A4 |
| ATOM | 2588 | CB  | ARG | 371 | 24.430 | 11.405 | 20.437 | 1.00 | 0.00 | 3A4 |
| ATOM | 2589 | CG  | ARG | 371 | 23.944 | 12.828 | 20.099 | 1.00 | 0.00 | 3A4 |
| ATOM | 2590 | CD  | ARG | 371 | 25.049 | 13.888 | 20.216 | 1.00 | 0.00 | 3A4 |
| ATOM | 2591 | NE  | ARG | 371 | 24.503 | 15.208 | 19.738 | 1.00 | 0.00 | 3A4 |
| ATOM | 2592 | CZ  | ARG | 371 | 25.012 | 16.428 | 20.108 | 1.00 | 0.00 | 3A4 |
| ATOM | 2593 | NH1 | ARG | 371 | 24.468 | 17.561 | 19.575 | 1.00 | 0.00 | 3A4 |
| ATOM | 2594 | NH2 | ARG | 371 | 26.049 | 16.546 | 20.988 | 1.00 | 0.00 | 3A4 |
| ATOM | 2595 | C   | ARG | 371 | 22.333 | 10.392 | 21.438 | 1.00 | 0.00 | 3A4 |
| ATOM | 2596 | O   | ARG | 371 | 21.181 | 10.760 | 21.216 | 1.00 | 0.00 | 3A4 |
| ATOM | 2597 | N   | LEU | 372 | 22.776 | 10.045 | 22.692 | 1.00 | 0.00 | 3A4 |
| ATOM | 2598 | CA  | LEU | 372 | 22.016 | 9.951  | 23.936 | 1.00 | 0.00 | 3A4 |
| ATOM | 2599 | CB  | LEU | 372 | 21.964 | 8.482  | 24.512 | 1.00 | 0.00 | 3A4 |
| ATOM | 2600 | CG  | LEU | 372 | 21.345 | 7.343  | 23.661 | 1.00 | 0.00 | 3A4 |
| ATOM | 2601 | CD1 | LEU | 372 | 19.908 | 7.641  | 23.227 | 1.00 | 0.00 | 3A4 |
| ATOM | 2602 | CD2 | LEU | 372 | 22.216 | 6.816  | 22.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 2603 | C   | LEU | 372 | 22.693 | 10.771 | 25.005 | 1.00 | 0.00 | 3A4 |
| ATOM | 2604 | O   | LEU | 372 | 23.899 | 11.003 | 24.975 | 1.00 | 0.00 | 3A4 |
| ATOM | 2605 | N   | GLU | 373 | 21.900 | 11.155 | 26.021 | 1.00 | 0.00 | 3A4 |
| ATOM | 2606 | CA  | GLU | 373 | 22.322 | 11.807 | 27.237 | 1.00 | 0.00 | 3A4 |
| ATOM | 2607 | CB  | GLU | 373 | 22.131 | 13.344 | 27.172 | 1.00 | 0.00 | 3A4 |
| ATOM | 2608 | CG  | GLU | 373 | 23.197 | 14.057 | 26.329 | 1.00 | 0.00 | 3A4 |
| ATOM | 2609 | CD  | GLU | 373 | 23.009 | 15.577 | 26.343 | 1.00 | 0.00 | 3A4 |
| ATOM | 2610 | OE1 | GLU | 373 | 23.722 | 16.250 | 25.553 | 1.00 | 0.00 | 3A4 |
| ATOM | 2611 | OE2 | GLU | 373 | 22.167 | 16.090 | 27.128 | 1.00 | 0.00 | 3A4 |
| ATOM | 2612 | C   | GLU | 373 | 21.466 | 11.241 | 28.351 | 1.00 | 0.00 | 3A4 |
| ATOM | 2613 | O   | GLU | 373 | 20.387 | 10.695 | 28.121 | 1.00 | 0.00 | 3A4 |
| ATOM | 2614 | N   | ARG | 374 | 21.930 | 11.386 | 29.612 | 1.00 | 0.00 | 3A4 |
| ATOM | 2615 | CA  | ARG | 374 | 21.138 | 11.043 | 30.774 | 1.00 | 0.00 | 3A4 |
| ATOM | 2616 | CB  | ARG | 374 | 21.532 | 9.678  | 31.420 | 1.00 | 0.00 | 3A4 |
| ATOM | 2617 | CG  | ARG | 374 | 22.371 | 9.595  | 32.715 | 1.00 | 0.00 | 3A4 |
| ATOM | 2618 | CD  | ARG | 374 | 21.558 | 9.546  | 34.018 | 1.00 | 0.00 | 3A4 |
| ATOM | 2619 | NE  | ARG | 374 | 22.476 | 9.916  | 35.152 | 1.00 | 0.00 | 3A4 |
| ATOM | 2620 | CZ  | ARG | 374 | 22.249 | 9.595  | 36.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 2621 | NH1 | ARG | 374 | 23.147 | 10.010 | 37.405 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2622 | NH2 | ARG | 374 | 21.156 | 8.879  | 36.860 | 1.00 | 0.00 | 3A4 |
| ATOM | 2623 | C   | ARG | 374 | 21.272 | 12.200 | 31.721 | 1.00 | 0.00 | 3A4 |
| ATOM | 2624 | O   | ARG | 374 | 22.360 | 12.720 | 31.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 2625 | N   | VAL | 375 | 20.152 | 12.629 | 32.340 | 1.00 | 0.00 | 3A4 |
| ATOM | 2626 | CA  | VAL | 375 | 20.085 | 13.742 | 33.272 | 1.00 | 0.00 | 3A4 |
| ATOM | 2627 | CB  | VAL | 375 | 18.651 | 14.239 | 33.344 | 1.00 | 0.00 | 3A4 |
| ATOM | 2628 | CG1 | VAL | 375 | 18.283 | 15.175 | 34.420 | 1.00 | 0.00 | 3A4 |
| ATOM | 2629 | CG2 | VAL | 375 | 18.394 | 14.888 | 31.964 | 1.00 | 0.00 | 3A4 |
| ATOM | 2630 | C   | VAL | 375 | 20.606 | 13.314 | 34.625 | 1.00 | 0.00 | 3A4 |
| ATOM | 2631 | O   | VAL | 375 | 20.173 | 12.325 | 35.197 | 1.00 | 0.00 | 3A4 |
| ATOM | 2632 | N   | CYS | 376 | 21.593 | 14.058 | 35.166 | 1.00 | 0.00 | 3A4 |
| ATOM | 2633 | CA  | CYS | 376 | 22.269 | 13.722 | 36.404 | 1.00 | 0.00 | 3A4 |
| ATOM | 2634 | CB  | CYS | 376 | 23.708 | 14.284 | 36.408 | 1.00 | 0.00 | 3A4 |
| ATOM | 2635 | SG  | CYS | 376 | 24.721 | 13.423 | 35.165 | 1.00 | 0.00 | 3A4 |
| ATOM | 2636 | C   | CYS | 376 | 21.525 | 14.230 | 37.618 | 1.00 | 0.00 | 3A4 |
| ATOM | 2637 | O   | CYS | 376 | 21.699 | 13.713 | 38.720 | 1.00 | 0.00 | 3A4 |
| ATOM | 2638 | N   | LYS | 377 | 20.691 | 15.268 | 37.426 | 1.00 | 0.00 | 3A4 |
| ATOM | 2639 | CA  | LYS | 377 | 19.982 | 15.944 | 38.480 | 1.00 | 0.00 | 3A4 |
| ATOM | 2640 | CB  | LYS | 377 | 20.773 | 17.167 | 38.996 | 1.00 | 0.00 | 3A4 |
| ATOM | 2641 | CG  | LYS | 377 | 22.008 | 16.876 | 39.867 | 1.00 | 0.00 | 3A4 |
| ATOM | 2642 | CD  | LYS | 377 | 21.695 | 16.179 | 41.198 | 1.00 | 0.00 | 3A4 |
| ATOM | 2643 | CE  | LYS | 377 | 22.947 | 15.957 | 42.056 | 1.00 | 0.00 | 3A4 |
| ATOM | 2644 | NZ  | LYS | 377 | 22.604 | 15.293 | 43.336 | 1.00 | 0.00 | 3A4 |
| ATOM | 2645 | C   | LYS | 377 | 18.735 | 16.448 | 37.827 | 1.00 | 0.00 | 3A4 |
| ATOM | 2646 | O   | LYS | 377 | 18.689 | 16.603 | 36.617 | 1.00 | 0.00 | 3A4 |
| ATOM | 2647 | N   | LYS | 378 | 17.690 | 16.839 | 38.593 | 1.00 | 0.00 | 3A4 |
| ATOM | 2648 | CA  | LYS | 378 | 16.465 | 17.414 | 38.063 | 1.00 | 0.00 | 3A4 |
| ATOM | 2649 | CB  | LYS | 378 | 15.419 | 17.607 | 39.177 | 1.00 | 0.00 | 3A4 |
| ATOM | 2650 | CG  | LYS | 378 | 15.088 | 16.287 | 39.895 | 1.00 | 0.00 | 3A4 |
| ATOM | 2651 | CD  | LYS | 378 | 14.017 | 16.418 | 40.984 | 1.00 | 0.00 | 3A4 |
| ATOM | 2652 | CE  | LYS | 378 | 13.613 | 15.082 | 41.625 | 1.00 | 0.00 | 3A4 |
| ATOM | 2653 | NZ  | LYS | 378 | 14.747 | 14.462 | 42.352 | 1.00 | 0.00 | 3A4 |
| ATOM | 2654 | C   | LYS | 378 | 16.741 | 18.741 | 37.382 | 1.00 | 0.00 | 3A4 |
| ATOM | 2655 | O   | LYS | 378 | 17.545 | 19.524 | 37.877 | 1.00 | 0.00 | 3A4 |
| ATOM | 2656 | N   | ASP | 379 | 16.172 | 18.960 | 36.183 | 1.00 | 0.00 | 3A4 |
| ATOM | 2657 | CA  | ASP | 379 | 16.483 | 20.125 | 35.394 | 1.00 | 0.00 | 3A4 |
| ATOM | 2658 | CB  | ASP | 379 | 17.706 | 19.925 | 34.443 | 1.00 | 0.00 | 3A4 |
| ATOM | 2659 | CG  | ASP | 379 | 17.527 | 19.059 | 33.183 | 1.00 | 0.00 | 3A4 |
| ATOM | 2660 | OD1 | ASP | 379 | 17.455 | 17.817 | 33.330 | 1.00 | 0.00 | 3A4 |
| ATOM | 2661 | OD2 | ASP | 379 | 17.475 | 19.634 | 32.063 | 1.00 | 0.00 | 3A4 |
| ATOM | 2662 | C   | ASP | 379 | 15.250 | 20.543 | 34.652 | 1.00 | 0.00 | 3A4 |
| ATOM | 2663 | O   | ASP | 379 | 14.333 | 19.776 | 34.415 | 1.00 | 0.00 | 3A4 |
| ATOM | 2664 | N   | VAL | 380 | 15.216 | 21.819 | 34.247 | 1.00 | 0.00 | 3A4 |
| ATOM | 2665 | CA  | VAL | 380 | 14.098 | 22.398 | 33.548 | 1.00 | 0.00 | 3A4 |
| ATOM | 2666 | CB  | VAL | 380 | 13.450 | 23.491 | 34.376 | 1.00 | 0.00 | 3A4 |
| ATOM | 2667 | CG1 | VAL | 380 | 12.212 | 24.040 | 33.665 | 1.00 | 0.00 | 3A4 |
| ATOM | 2668 | CG2 | VAL | 380 | 13.057 | 22.943 | 35.763 | 1.00 | 0.00 | 3A4 |
| ATOM | 2669 | C   | VAL | 380 | 14.659 | 22.869 | 32.227 | 1.00 | 0.00 | 3A4 |
| ATOM | 2670 | O   | VAL | 380 | 15.521 | 23.743 | 32.201 | 1.00 | 0.00 | 3A4 |
| ATOM | 2671 | N   | GLU | 381 | 14.219 | 22.259 | 31.107 | 1.00 | 0.00 | 3A4 |
| ATOM | 2672 | CA  | GLU | 381 | 14.653 | 22.560 | 29.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 2673 | CB  | GLU | 381 | 15.044 | 21.298 | 28.989 | 1.00 | 0.00 | 3A4 |
| ATOM | 2674 | CG  | GLU | 381 | 15.995 | 21.611 | 27.810 | 1.00 | 0.00 | 3A4 |
| ATOM | 2675 | CD  | GLU | 381 | 16.331 | 20.375 | 26.965 | 1.00 | 0.00 | 3A4 |
| ATOM | 2676 | OE1 | GLU | 381 | 17.063 | 20.564 | 25.958 | 1.00 | 0.00 | 3A4 |
| ATOM | 2677 | OE2 | GLU | 381 | 15.873 | 19.246 | 27.284 | 1.00 | 0.00 | 3A4 |
| ATOM | 2678 | C   | GLU | 381 | 13.495 | 23.231 | 29.052 | 1.00 | 0.00 | 3A4 |
| ATOM | 2679 | O   | GLU | 381 | 12.355 | 22.802 | 29.042 | 1.00 | 0.00 | 3A4 |
| ATOM | 2680 | N   | ILE | 382 | 13.715 | 24.405 | 28.468 | 1.00 | 0.00 | 3A4 |
| ATOM | 2681 | CA  | ILE | 382 | 12.690 | 25.313 | 27.960 | 1.00 | 0.00 | 3A4 |
| ATOM | 2682 | CB  | ILE | 382 | 11.956 | 24.945 | 26.638 | 1.00 | 0.00 | 3A4 |
| ATOM | 2683 | CG2 | ILE | 382 | 10.525 | 25.549 | 26.472 | 1.00 | 0.00 | 3A4 |
| ATOM | 2684 | CG1 | ILE | 382 | 12.874 | 25.434 | 25.467 | 1.00 | 0.00 | 3A4 |
| ATOM | 2685 | CD  | ILE | 382 | 12.229 | 25.497 | 24.082 | 1.00 | 0.00 | 3A4 |
| ATOM | 2686 | C   | ILE | 382 | 11.919 | 25.809 | 29.163 | 1.00 | 0.00 | 3A4 |
| ATOM | 2687 | O   | ILE | 382 | 12.497 | 26.469 | 29.990 | 1.00 | 0.00 | 3A4 |
| ATOM | 2688 | N   | ASN | 383 | 10.722 | 25.435 | 29.490 | 1.00 | 0.00 | 3A4 |
| ATOM | 2689 | CA  | ASN | 383 | 10.349 | 25.838 | 30.866 | 1.00 | 0.00 | 3A4 |
| ATOM | 2690 | CB  | ASN | 383 | 9.806  | 27.330 | 30.959 | 1.00 | 0.00 | 3A4 |
| ATOM | 2691 | CG  | ASN | 383 | 9.693  | 27.860 | 32.407 | 1.00 | 0.00 | 3A4 |
| ATOM | 2692 | OD1 | ASN | 383 | 8.596  | 28.169 | 32.869 | 1.00 | 0.00 | 3A4 |
| ATOM | 2693 | ND2 | ASN | 383 | 10.843 | 27.967 | 33.129 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2694 | C   | ASN | 383 | 9.349  | 24.945 | 31.284 | 1.00 | 0.00 | 3A4 |
| ATOM | 2695 | O   | ASN | 383 | 8.160  | 25.107 | 30.993 | 1.00 | 0.00 | 3A4 |
| ATOM | 2696 | N   | GLY | 384 | 9.485  | 23.892 | 32.102 | 1.00 | 0.00 | 3A4 |
| ATOM | 2697 | CA  | GLY | 384 | 8.315  | 22.984 | 32.156 | 1.00 | 0.00 | 3A4 |
| ATOM | 2698 | C   | GLY | 384 | 8.276  | 22.292 | 30.798 | 1.00 | 0.00 | 3A4 |
| ATOM | 2699 | O   | GLY | 384 | 7.285  | 21.764 | 30.297 | 1.00 | 0.00 | 3A4 |
| ATOM | 2700 | N   | MET | 385 | 9.600  | 22.252 | 30.331 | 1.00 | 0.00 | 3A4 |
| ATOM | 2701 | CA  | MET | 385 | 9.904  | 20.858 | 30.491 | 1.00 | 0.00 | 3A4 |
| ATOM | 2702 | CB  | MET | 385 | 10.648 | 20.273 | 29.245 | 1.00 | 0.00 | 3A4 |
| ATOM | 2703 | CG  | MET | 385 | 10.078 | 18.932 | 28.749 | 1.00 | 0.00 | 3A4 |
| ATOM | 2704 | SD  | MET | 385 | 10.271 | 17.522 | 29.885 | 1.00 | 0.00 | 3A4 |
| ATOM | 2705 | CE  | MET | 385 | 8.674  | 16.747 | 29.504 | 1.00 | 0.00 | 3A4 |
| ATOM | 2706 | C   | MET | 385 | 10.673 | 20.574 | 31.772 | 1.00 | 0.00 | 3A4 |
| ATOM | 2707 | O   | MET | 385 | 11.823 | 20.957 | 31.867 | 1.00 | 0.00 | 3A4 |
| ATOM | 2708 | N   | PHE | 386 | 10.077 | 19.903 | 32.767 | 1.00 | 0.00 | 3A4 |
| ATOM | 2709 | CA  | PHE | 386 | 10.786 | 19.416 | 33.933 | 1.00 | 0.00 | 3A4 |
| ATOM | 2710 | CB  | PHE | 386 | 9.854  | 19.471 | 35.160 | 1.00 | 0.00 | 3A4 |
| ATOM | 2711 | CG  | PHE | 386 | 10.561 | 19.327 | 36.492 | 1.00 | 0.00 | 3A4 |
| ATOM | 2712 | CD1 | PHE | 386 | 10.905 | 20.467 | 37.242 | 1.00 | 0.00 | 3A4 |
| ATOM | 2713 | CD2 | PHE | 386 | 10.861 | 18.057 | 37.026 | 1.00 | 0.00 | 3A4 |
| ATOM | 2714 | CE1 | PHE | 386 | 11.556 | 20.349 | 38.477 | 1.00 | 0.00 | 3A4 |
| ATOM | 2715 | CE2 | PHE | 386 | 11.512 | 17.931 | 38.260 | 1.00 | 0.00 | 3A4 |
| ATOM | 2716 | CZ  | PHE | 386 | 11.859 | 19.080 | 38.985 | 1.00 | 0.00 | 3A4 |
| ATOM | 2717 | C   | PHE | 386 | 11.245 | 17.997 | 33.650 | 1.00 | 0.00 | 3A4 |
| ATOM | 2718 | O   | PHE | 386 | 10.434 | 17.097 | 33.442 | 1.00 | 0.00 | 3A4 |
| ATOM | 2719 | N   | ILE | 387 | 12.579 | 17.797 | 33.622 | 1.00 | 0.00 | 3A4 |
| ATOM | 2720 | CA  | ILE | 387 | 13.234 | 16.542 | 33.348 | 1.00 | 0.00 | 3A4 |
| ATOM | 2721 | CB  | ILE | 387 | 14.381 | 16.682 | 32.335 | 1.00 | 0.00 | 3A4 |
| ATOM | 2722 | CG2 | ILE | 387 | 14.760 | 15.256 | 31.874 | 1.00 | 0.00 | 3A4 |
| ATOM | 2723 | CG1 | ILE | 387 | 13.940 | 17.566 | 31.142 | 1.00 | 0.00 | 3A4 |
| ATOM | 2724 | CD  | ILE | 387 | 14.996 | 17.732 | 30.052 | 1.00 | 0.00 | 3A4 |
| ATOM | 2725 | C   | ILE | 387 | 13.712 | 16.037 | 34.699 | 1.00 | 0.00 | 3A4 |
| ATOM | 2726 | O   | ILE | 387 | 14.542 | 16.701 | 35.311 | 1.00 | 0.00 | 3A4 |
| ATOM | 2727 | N   | PRO | 388 | 13.230 | 14.898 | 35.231 | 1.00 | 0.00 | 3A4 |
| ATOM | 2728 | CA  | PRO | 388 | 13.741 | 14.297 | 36.449 | 1.00 | 0.00 | 3A4 |
| ATOM | 2729 | CD  | PRO | 388 | 11.827 | 14.522 | 35.038 | 1.00 | 0.00 | 3A4 |
| ATOM | 2730 | CB  | PRO | 388 | 12.685 | 13.264 | 36.864 | 1.00 | 0.00 | 3A4 |
| ATOM | 2731 | CG  | PRO | 388 | 11.381 | 13.833 | 36.327 | 1.00 | 0.00 | 3A4 |
| ATOM | 2732 | C   | PRO | 388 | 15.090 | 13.656 | 36.297 | 1.00 | 0.00 | 3A4 |
| ATOM | 2733 | O   | PRO | 388 | 15.481 | 13.246 | 35.212 | 1.00 | 0.00 | 3A4 |
| ATOM | 2734 | N   | LYS | 389 | 15.825 | 13.516 | 37.416 | 1.00 | 0.00 | 3A4 |
| ATOM | 2735 | CA  | LYS | 389 | 17.102 | 12.839 | 37.479 | 1.00 | 0.00 | 3A4 |
| ATOM | 2736 | CB  | LYS | 389 | 17.661 | 12.891 | 38.918 | 1.00 | 0.00 | 3A4 |
| ATOM | 2737 | CG  | LYS | 389 | 16.754 | 12.453 | 40.092 | 1.00 | 0.00 | 3A4 |
| ATOM | 2738 | CD  | LYS | 389 | 16.878 | 10.984 | 40.532 | 1.00 | 0.00 | 3A4 |
| ATOM | 2739 | CE  | LYS | 389 | 16.079 | 10.653 | 41.802 | 1.00 | 0.00 | 3A4 |
| ATOM | 2740 | NZ  | LYS | 389 | 14.624 | 10.849 | 41.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 2741 | C   | LYS | 389 | 16.984 | 11.412 | 37.009 | 1.00 | 0.00 | 3A4 |
| ATOM | 2742 | O   | LYS | 389 | 15.997 | 10.745 | 37.301 | 1.00 | 0.00 | 3A4 |
| ATOM | 2743 | N   | GLY | 390 | 17.932 | 10.973 | 36.172 | 1.00 | 0.00 | 3A4 |
| ATOM | 2744 | CA  | GLY | 390 | 17.963 | 9.654  | 35.593 | 1.00 | 0.00 | 3A4 |
| ATOM | 2745 | C   | GLY | 390 | 17.174 | 9.470  | 34.332 | 1.00 | 0.00 | 3A4 |
| ATOM | 2746 | O   | GLY | 390 | 17.046 | 8.351  | 33.839 | 1.00 | 0.00 | 3A4 |
| ATOM | 2747 | N   | TRP | 391 | 16.619 | 10.571 | 33.769 | 1.00 | 0.00 | 3A4 |
| ATOM | 2748 | CA  | TRP | 391 | 15.850 | 10.544 | 32.546 | 1.00 | 0.00 | 3A4 |
| ATOM | 2749 | CB  | TRP | 391 | 14.930 | 11.760 | 32.448 | 1.00 | 0.00 | 3A4 |
| ATOM | 2750 | CG  | TRP | 391 | 13.571 | 11.608 | 33.100 | 1.00 | 0.00 | 3A4 |
| ATOM | 2751 | CD2 | TRP | 391 | 13.050 | 10.792 | 34.187 | 1.00 | 0.00 | 3A4 |
| ATOM | 2752 | CD1 | TRP | 391 | 12.458 | 12.068 | 32.439 | 1.00 | 0.00 | 3A4 |
| ATOM | 2753 | NE1 | TRP | 391 | 11.305 | 11.618 | 33.025 | 1.00 | 0.00 | 3A4 |
| ATOM | 2754 | CE2 | TRP | 391 | 11.634 | 10.839 | 34.102 | 1.00 | 0.00 | 3A4 |
| ATOM | 2755 | CE3 | TRP | 391 | 13.655 | 10.032 | 35.188 | 1.00 | 0.00 | 3A4 |
| ATOM | 2756 | CZ2 | TRP | 391 | 10.825 | 10.153 | 35.005 | 1.00 | 0.00 | 3A4 |
| ATOM | 2757 | CZ3 | TRP | 391 | 12.843 | 9.345  | 36.102 | 1.00 | 0.00 | 3A4 |
| ATOM | 2758 | CH2 | TRP | 391 | 11.446 | 9.404  | 36.011 | 1.00 | 0.00 | 3A4 |
| ATOM | 2759 | C   | TRP | 391 | 16.783 | 10.563 | 31.369 | 1.00 | 0.00 | 3A4 |
| ATOM | 2760 | O   | TRP | 391 | 17.769 | 11.289 | 31.371 | 1.00 | 0.00 | 3A4 |
| ATOM | 2761 | N   | VAL | 392 | 16.466 | 9.736  | 30.350 | 1.00 | 0.00 | 3A4 |
| ATOM | 2762 | CA  | VAL | 392 | 17.263 | 9.564  | 29.159 | 1.00 | 0.00 | 3A4 |
| ATOM | 2763 | CB  | VAL | 392 | 17.270 | 8.105  | 28.700 | 1.00 | 0.00 | 3A4 |
| ATOM | 2764 | CG1 | VAL | 392 | 17.957 | 7.898  | 27.322 | 1.00 | 0.00 | 3A4 |
| ATOM | 2765 | CG2 | VAL | 392 | 17.984 | 7.270  | 29.787 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2766 | C   | VAL | 392 | 16.723 | 10.497 | 28.110 | 1.00 | 0.00 | 3A4 |
| ATOM | 2767 | O   | VAL | 392 | 15.519 | 10.598 | 27.908 | 1.00 | 0.00 | 3A4 |
| ATOM | 2768 | N   | VAL | 393 | 17.636 | 11.234 | 27.453 | 1.00 | 0.00 | 3A4 |
| ATOM | 2769 | CA  | VAL | 393 | 17.333 | 12.226 | 26.455 | 1.00 | 0.00 | 3A4 |
| ATOM | 2770 | CB  | VAL | 393 | 17.828 | 13.610 | 26.868 | 1.00 | 0.00 | 3A4 |
| ATOM | 2771 | CG1 | VAL | 393 | 17.556 | 14.652 | 25.780 | 1.00 | 0.00 | 3A4 |
| ATOM | 2772 | CG2 | VAL | 393 | 17.145 | 14.023 | 28.194 | 1.00 | 0.00 | 3A4 |
| ATOM | 2773 | C   | VAL | 393 | 17.993 | 11.735 | 25.192 | 1.00 | 0.00 | 3A4 |
| ATOM | 2774 | O   | VAL | 393 | 19.147 | 11.327 | 25.196 | 1.00 | 0.00 | 3A4 |
| ATOM | 2775 | N   | MET | 394 | 17.251 | 11.776 | 24.072 | 1.00 | 0.00 | 3A4 |
| ATOM | 2776 | CA  | MET | 394 | 17.726 | 11.439 | 22.757 | 1.00 | 0.00 | 3A4 |
| ATOM | 2777 | CB  | MET | 394 | 16.799 | 10.393 | 22.065 | 1.00 | 0.00 | 3A4 |
| ATOM | 2778 | CG  | MET | 394 | 16.558 | 9.106  | 22.860 | 1.00 | 0.00 | 3A4 |
| ATOM | 2779 | SD  | MET | 394 | 15.673 | 7.800  | 21.946 | 1.00 | 0.00 | 3A4 |
| ATOM | 2780 | CE  | MET | 394 | 16.910 | 7.426  | 20.666 | 1.00 | 0.00 | 3A4 |
| ATOM | 2781 | C   | MET | 394 | 17.772 | 12.724 | 21.991 | 1.00 | 0.00 | 3A4 |
| ATOM | 2782 | O   | MET | 394 | 16.799 | 13.464 | 21.947 | 1.00 | 0.00 | 3A4 |
| ATOM | 2783 | N   | ILE | 395 | 18.916 | 13.023 | 21.347 | 1.00 | 0.00 | 3A4 |
| ATOM | 2784 | CA  | ILE | 395 | 19.139 | 14.208 | 20.554 | 1.00 | 0.00 | 3A4 |
| ATOM | 2785 | CB  | ILE | 395 | 20.476 | 14.837 | 20.956 | 1.00 | 0.00 | 3A4 |
| ATOM | 2786 | CG2 | ILE | 395 | 21.095 | 15.840 | 19.965 | 1.00 | 0.00 | 3A4 |
| ATOM | 2787 | CG1 | ILE | 395 | 20.413 | 15.442 | 22.374 | 1.00 | 0.00 | 3A4 |
| ATOM | 2788 | CD  | ILE | 395 | 20.802 | 14.496 | 23.518 | 1.00 | 0.00 | 3A4 |
| ATOM | 2789 | C   | ILE | 395 | 19.146 | 13.747 | 19.102 | 1.00 | 0.00 | 3A4 |
| ATOM | 2790 | O   | ILE | 395 | 20.160 | 13.239 | 18.627 | 1.00 | 0.00 | 3A4 |
| ATOM | 2791 | N   | PRO | 396 | 18.048 | 13.907 | 18.342 | 1.00 | 0.00 | 3A4 |
| ATOM | 2792 | CA  | PRO | 396 | 18.027 | 13.792 | 16.906 | 1.00 | 0.00 | 3A4 |
| ATOM | 2793 | CD  | PRO | 396 | 16.755 | 13.448 | 18.870 | 1.00 | 0.00 | 3A4 |
| ATOM | 2794 | CB  | PRO | 396 | 16.531 | 13.829 | 16.546 | 1.00 | 0.00 | 3A4 |
| ATOM | 2795 | CG  | PRO | 396 | 15.857 | 13.097 | 17.687 | 1.00 | 0.00 | 3A4 |
| ATOM | 2796 | C   | PRO | 396 | 18.776 | 14.889 | 16.173 | 1.00 | 0.00 | 3A4 |
| ATOM | 2797 | O   | PRO | 396 | 18.239 | 15.950 | 15.861 | 1.00 | 0.00 | 3A4 |
| ATOM | 2798 | N   | SER | 397 | 20.048 | 14.601 | 15.825 | 1.00 | 0.00 | 3A4 |
| ATOM | 2799 | CA  | SER | 397 | 20.904 | 15.470 | 15.055 | 1.00 | 0.00 | 3A4 |
| ATOM | 2800 | CB  | SER | 397 | 22.360 | 14.989 | 15.079 | 1.00 | 0.00 | 3A4 |
| ATOM | 2801 | OG  | SER | 397 | 22.500 | 13.601 | 14.800 | 1.00 | 0.00 | 3A4 |
| ATOM | 2802 | C   | SER | 397 | 20.417 | 15.595 | 13.635 | 1.00 | 0.00 | 3A4 |
| ATOM | 2803 | O   | SER | 397 | 20.522 | 16.640 | 13.023 | 1.00 | 0.00 | 3A4 |
| ATOM | 2804 | N   | TYR | 398 | 19.766 | 14.539 | 13.106 | 1.00 | 0.00 | 3A4 |
| ATOM | 2805 | CA  | TYR | 398 | 19.026 | 14.496 | 11.862 | 1.00 | 0.00 | 3A4 |
| ATOM | 2806 | CB  | TYR | 398 | 18.323 | 13.079 | 11.799 | 1.00 | 0.00 | 3A4 |
| ATOM | 2807 | CG  | TYR | 398 | 18.447 | 12.353 | 10.483 | 1.00 | 0.00 | 3A4 |
| ATOM | 2808 | CD1 | TYR | 398 | 19.004 | 11.056 | 10.456 | 1.00 | 0.00 | 3A4 |
| ATOM | 2809 | CD2 | TYR | 398 | 18.041 | 12.935 | 9.266  | 1.00 | 0.00 | 3A4 |
| ATOM | 2810 | CE1 | TYR | 398 | 19.153 | 10.357 | 9.251  | 1.00 | 0.00 | 3A4 |
| ATOM | 2811 | CE2 | TYR | 398 | 18.216 | 12.249 | 8.058  | 1.00 | 0.00 | 3A4 |
| ATOM | 2812 | CZ  | TYR | 398 | 18.763 | 10.958 | 8.048  | 1.00 | 0.00 | 3A4 |
| ATOM | 2813 | OH  | TYR | 398 | 18.924 | 10.266 | 6.829  | 1.00 | 0.00 | 3A4 |
| ATOM | 2814 | C   | TYR | 398 | 17.923 | 15.540 | 11.741 | 1.00 | 0.00 | 3A4 |
| ATOM | 2815 | O   | TYR | 398 | 17.730 | 16.207 | 10.728 | 1.00 | 0.00 | 3A4 |
| ATOM | 2816 | N   | ALA | 399 | 17.184 | 15.730 | 12.853 | 1.00 | 0.00 | 3A4 |
| ATOM | 2817 | CA  | ALA | 399 | 16.116 | 16.686 | 12.969 | 1.00 | 0.00 | 3A4 |
| ATOM | 2818 | CB  | ALA | 399 | 15.263 | 16.409 | 14.206 | 1.00 | 0.00 | 3A4 |
| ATOM | 2819 | C   | ALA | 399 | 16.594 | 18.122 | 13.028 | 1.00 | 0.00 | 3A4 |
| ATOM | 2820 | O   | ALA | 399 | 15.939 | 19.008 | 12.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 2821 | N   | LEU | 400 | 17.795 | 18.377 | 13.599 | 1.00 | 0.00 | 3A4 |
| ATOM | 2822 | CA  | LEU | 400 | 18.426 | 19.687 | 13.645 | 1.00 | 0.00 | 3A4 |
| ATOM | 2823 | CB  | LEU | 400 | 19.762 | 19.647 | 14.448 | 1.00 | 0.00 | 3A4 |
| ATOM | 2824 | CG  | LEU | 400 | 19.694 | 19.664 | 15.956 | 1.00 | 0.00 | 3A4 |
| ATOM | 2825 | CD1 | LEU | 400 | 20.663 | 20.773 | 16.433 | 1.00 | 0.00 | 3A4 |
| ATOM | 2826 | CD2 | LEU | 400 | 18.244 | 19.759 | 16.433 | 1.00 | 0.00 | 3A4 |
| ATOM | 2827 | C   | LEU | 400 | 18.832 | 20.202 | 12.285 | 1.00 | 0.00 | 3A4 |
| ATOM | 2828 | O   | LEU | 400 | 18.639 | 21.368 | 11.954 | 1.00 | 0.00 | 3A4 |
| ATOM | 2829 | N   | HIS | 401 | 19.402 | 19.298 | 11.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 2830 | CA  | HIS | 401 | 19.852 | 19.556 | 10.124 | 1.00 | 0.00 | 3A4 |
| ATOM | 2831 | ND1 | HIS | 401 | 22.332 | 16.943 | 10.714 | 1.00 | 0.00 | 3A4 |
| ATOM | 2832 | CG  | HIS | 401 | 21.917 | 18.117 | 10.143 | 1.00 | 0.00 | 3A4 |
| ATOM | 2833 | CB  | HIS | 401 | 20.572 | 18.319 | 9.559  | 1.00 | 0.00 | 3A4 |
| ATOM | 2834 | NE2 | HIS | 401 | 24.123 | 18.219 | 10.505 | 1.00 | 0.00 | 3A4 |
| ATOM | 2835 | CD2 | HIS | 401 | 23.023 | 18.893 | 10.033 | 1.00 | 0.00 | 3A4 |
| ATOM | 2836 | CE1 | HIS | 401 | 23.659 | 17.057 | 10.914 | 1.00 | 0.00 | 3A4 |
| ATOM | 2837 | C   | HIS | 401 | 18.745 | 19.836 | 9.125  | 1.00 | 0.00 | 3A4 |



|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2838 | O   | HIS | 401 | 18.970 | 20.398 | 8.056  | 1.00 | 0.00 | 3A4 |
| ATOM | 2839 | N   | ARG | 402 | 17.513 | 19.410 | 9.474  | 1.00 | 0.00 | 3A4 |
| ATOM | 2840 | CA  | ARG | 402 | 16.350 | 19.558 | 8.644  | 1.00 | 0.00 | 3A4 |
| ATOM | 2841 | CB  | ARG | 402 | 15.632 | 18.220 | 8.410  | 1.00 | 0.00 | 3A4 |
| ATOM | 2842 | CG  | ARG | 402 | 16.476 | 17.220 | 7.607  | 1.00 | 0.00 | 3A4 |
| ATOM | 2843 | CD  | ARG | 402 | 15.663 | 15.992 | 7.176  | 1.00 | 0.00 | 3A4 |
| ATOM | 2844 | NE  | ARG | 402 | 16.519 | 15.105 | 6.308  | 1.00 | 0.00 | 3A4 |
| ATOM | 2845 | CZ  | ARG | 402 | 16.028 | 14.373 | 5.254  | 1.00 | 0.00 | 3A4 |
| ATOM | 2846 | NH1 | ARG | 402 | 16.860 | 13.518 | 4.593  | 1.00 | 0.00 | 3A4 |
| ATOM | 2847 | NH2 | ARG | 402 | 14.725 | 14.465 | 4.853  | 1.00 | 0.00 | 3A4 |
| ATOM | 2848 | C   | ARG | 402 | 15.378 | 20.553 | 9.211  | 1.00 | 0.00 | 3A4 |
| ATOM | 2849 | O   | ARG | 402 | 14.224 | 20.625 | 8.790  | 1.00 | 0.00 | 3A4 |
| ATOM | 2850 | N   | ASP | 403 | 15.839 | 21.391 | 10.171 | 1.00 | 0.00 | 3A4 |
| ATOM | 2851 | CA  | ASP | 403 | 15.031 | 22.422 | 10.772 | 1.00 | 0.00 | 3A4 |
| ATOM | 2852 | CB  | ASP | 403 | 15.642 | 22.973 | 12.085 | 1.00 | 0.00 | 3A4 |
| ATOM | 2853 | CG  | ASP | 403 | 14.530 | 23.734 | 12.847 | 1.00 | 0.00 | 3A4 |
| ATOM | 2854 | OD1 | ASP | 403 | 14.116 | 24.806 | 12.394 | 1.00 | 0.00 | 3A4 |
| ATOM | 2855 | OD2 | ASP | 403 | 13.981 | 23.160 | 13.823 | 1.00 | 0.00 | 3A4 |
| ATOM | 2856 | C   | ASP | 403 | 14.822 | 23.549 | 9.771  | 1.00 | 0.00 | 3A4 |
| ATOM | 2857 | O   | ASP | 403 | 15.805 | 24.148 | 9.348  | 1.00 | 0.00 | 3A4 |
| ATOM | 2858 | N   | PRO | 404 | 13.575 | 23.872 | 9.387  | 1.00 | 0.00 | 3A4 |
| ATOM | 2859 | CA  | PRO | 404 | 13.256 | 24.866 | 8.377  | 1.00 | 0.00 | 3A4 |
| ATOM | 2860 | CD  | PRO | 404 | 12.350 | 23.288 | 9.945  | 1.00 | 0.00 | 3A4 |
| ATOM | 2861 | CB  | PRO | 404 | 11.749 | 24.727 | 8.133  | 1.00 | 0.00 | 3A4 |
| ATOM | 2862 | CG  | PRO | 404 | 11.195 | 24.161 | 9.445  | 1.00 | 0.00 | 3A4 |
| ATOM | 2863 | C   | PRO | 404 | 13.582 | 26.287 | 8.784  | 1.00 | 0.00 | 3A4 |
| ATOM | 2864 | O   | PRO | 404 | 13.786 | 27.122 | 7.915  | 1.00 | 0.00 | 3A4 |
| ATOM | 2865 | N   | LYS | 405 | 13.702 | 26.594 | 10.092 | 1.00 | 0.00 | 3A4 |
| ATOM | 2866 | CA  | LYS | 405 | 14.102 | 27.890 | 10.588 | 1.00 | 0.00 | 3A4 |
| ATOM | 2867 | CB  | LYS | 405 | 13.708 | 28.082 | 12.078 | 1.00 | 0.00 | 3A4 |
| ATOM | 2868 | CG  | LYS | 405 | 12.230 | 27.779 | 12.361 | 1.00 | 0.00 | 3A4 |
| ATOM | 2869 | CD  | LYS | 405 | 11.862 | 27.931 | 13.843 | 1.00 | 0.00 | 3A4 |
| ATOM | 2870 | CE  | LYS | 405 | 10.437 | 27.465 | 14.181 | 1.00 | 0.00 | 3A4 |
| ATOM | 2871 | NZ  | LYS | 405 | 9.420  | 28.274 | 13.467 | 1.00 | 0.00 | 3A4 |
| ATOM | 2872 | C   | LYS | 405 | 15.589 | 28.111 | 10.451 | 1.00 | 0.00 | 3A4 |
| ATOM | 2873 | O   | LYS | 405 | 16.040 | 29.247 | 10.435 | 1.00 | 0.00 | 3A4 |
| ATOM | 2874 | N   | TYR | 406 | 16.387 | 27.031 | 10.326 | 1.00 | 0.00 | 3A4 |
| ATOM | 2875 | CA  | TYR | 406 | 17.828 | 27.082 | 10.196 | 1.00 | 0.00 | 3A4 |
| ATOM | 2876 | CB  | TYR | 406 | 18.501 | 25.978 | 11.073 | 1.00 | 0.00 | 3A4 |
| ATOM | 2877 | CG  | TYR | 406 | 18.818 | 26.481 | 12.466 | 1.00 | 0.00 | 3A4 |
| ATOM | 2878 | CD1 | TYR | 406 | 17.845 | 27.049 | 13.316 | 1.00 | 0.00 | 3A4 |
| ATOM | 2879 | CD2 | TYR | 406 | 20.123 | 26.324 | 12.973 | 1.00 | 0.00 | 3A4 |
| ATOM | 2880 | CE1 | TYR | 406 | 18.180 | 27.502 | 14.601 | 1.00 | 0.00 | 3A4 |
| ATOM | 2881 | CE2 | TYR | 406 | 20.465 | 26.758 | 14.261 | 1.00 | 0.00 | 3A4 |
| ATOM | 2882 | CZ  | TYR | 406 | 19.493 | 27.354 | 15.076 | 1.00 | 0.00 | 3A4 |
| ATOM | 2883 | OH  | TYR | 406 | 19.831 | 27.781 | 16.379 | 1.00 | 0.00 | 3A4 |
| ATOM | 2884 | C   | TYR | 406 | 18.238 | 26.911 | 8.742  | 1.00 | 0.00 | 3A4 |
| ATOM | 2885 | O   | TYR | 406 | 19.185 | 27.556 | 8.293  | 1.00 | 0.00 | 3A4 |
| ATOM | 2886 | N   | TRP | 407 | 17.542 | 26.030 | 7.986  | 1.00 | 0.00 | 3A4 |
| ATOM | 2887 | CA  | TRP | 407 | 17.869 | 25.728 | 6.609  | 1.00 | 0.00 | 3A4 |
| ATOM | 2888 | CB  | TRP | 407 | 18.602 | 24.364 | 6.460  | 1.00 | 0.00 | 3A4 |
| ATOM | 2889 | CG  | TRP | 407 | 19.890 | 24.534 | 5.666  | 1.00 | 0.00 | 3A4 |
| ATOM | 2890 | CD2 | TRP | 407 | 20.082 | 24.159 | 4.293  | 1.00 | 0.00 | 3A4 |
| ATOM | 2891 | CD1 | TRP | 407 | 21.050 | 25.141 | 6.063  | 1.00 | 0.00 | 3A4 |
| ATOM | 2892 | NE1 | TRP | 407 | 21.981 | 25.110 | 5.052  | 1.00 | 0.00 | 3A4 |
| ATOM | 2893 | CE2 | TRP | 407 | 21.405 | 24.521 | 3.948  | 1.00 | 0.00 | 3A4 |
| ATOM | 2894 | CE3 | TRP | 407 | 19.231 | 23.566 | 3.365  | 1.00 | 0.00 | 3A4 |
| ATOM | 2895 | CZ2 | TRP | 407 | 21.902 | 24.280 | 2.673  | 1.00 | 0.00 | 3A4 |
| ATOM | 2896 | CZ3 | TRP | 407 | 19.728 | 23.326 | 2.076  | 1.00 | 0.00 | 3A4 |
| ATOM | 2897 | CH2 | TRP | 407 | 21.046 | 23.678 | 1.741  | 1.00 | 0.00 | 3A4 |
| ATOM | 2898 | C   | TRP | 407 | 16.592 | 25.684 | 5.809  | 1.00 | 0.00 | 3A4 |
| ATOM | 2899 | O   | TRP | 407 | 15.735 | 24.831 | 6.029  | 1.00 | 0.00 | 3A4 |
| ATOM | 2900 | N   | THR | 408 | 16.454 | 26.581 | 4.791  | 1.00 | 0.00 | 3A4 |
| ATOM | 2901 | CA  | THR | 408 | 15.311 | 26.691 | 3.895  | 1.00 | 0.00 | 3A4 |
| ATOM | 2902 | CB  | THR | 408 | 15.211 | 28.071 | 3.263  | 1.00 | 0.00 | 3A4 |
| ATOM | 2903 | OG1 | THR | 408 | 16.432 | 28.505 | 2.662  | 1.00 | 0.00 | 3A4 |
| ATOM | 2904 | CG2 | THR | 408 | 14.818 | 29.070 | 4.376  | 1.00 | 0.00 | 3A4 |
| ATOM | 2905 | C   | THR | 408 | 15.392 | 25.598 | 2.839  | 1.00 | 0.00 | 3A4 |
| ATOM | 2906 | O   | THR | 408 | 16.472 | 25.245 | 2.376  | 1.00 | 0.00 | 3A4 |
| ATOM | 2907 | N   | GLU | 409 | 14.235 | 24.987 | 2.499  | 1.00 | 0.00 | 3A4 |
| ATOM | 2908 | CA  | GLU | 409 | 14.103 | 23.803 | 1.664  | 1.00 | 0.00 | 3A4 |
| ATOM | 2909 | CB  | GLU | 409 | 14.330 | 24.118 | 0.167  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2910 | CG  | GLU | 409 | 13.370 | 25.190 | -0.379 | 1.00 | 0.00 | 3A4 |
| ATOM | 2911 | CD  | GLU | 409 | 13.625 | 25.385 | -1.878 | 1.00 | 0.00 | 3A4 |
| ATOM | 2912 | OE1 | GLU | 409 | 12.698 | 25.099 | -2.683 | 1.00 | 0.00 | 3A4 |
| ATOM | 2913 | OE2 | GLU | 409 | 14.752 | 25.821 | -2.236 | 1.00 | 0.00 | 3A4 |
| ATOM | 2914 | C   | GLU | 409 | 15.001 | 22.657 | 2.097  | 1.00 | 0.00 | 3A4 |
| ATOM | 2915 | O   | GLU | 409 | 15.858 | 22.218 | 1.334  | 1.00 | 0.00 | 3A4 |
| ATOM | 2916 | N   | PRO | 410 | 14.886 | 22.233 | 3.369  | 1.00 | 0.00 | 3A4 |
| ATOM | 2917 | CA  | PRO | 410 | 15.857 | 21.388 | 4.073  | 1.00 | 0.00 | 3A4 |
| ATOM | 2918 | CD  | PRO | 410 | 13.663 | 22.414 | 4.165  | 1.00 | 0.00 | 3A4 |
| ATOM | 2919 | CB  | PRO | 410 | 15.298 | 21.307 | 5.504  | 1.00 | 0.00 | 3A4 |
| ATOM | 2920 | CG  | PRO | 410 | 13.783 | 21.467 | 5.357  | 1.00 | 0.00 | 3A4 |
| ATOM | 2921 | C   | PRO | 410 | 16.013 | 20.007 | 3.463  | 1.00 | 0.00 | 3A4 |
| ATOM | 2922 | O   | PRO | 410 | 17.048 | 19.368 | 3.620  | 1.00 | 0.00 | 3A4 |
| ATOM | 2923 | N   | GLU | 411 | 15.001 | 19.530 | 2.723  | 1.00 | 0.00 | 3A4 |
| ATOM | 2924 | CA  | GLU | 411 | 15.007 | 18.249 | 2.086  | 1.00 | 0.00 | 3A4 |
| ATOM | 2925 | CB  | GLU | 411 | 13.575 | 17.671 | 2.041  | 1.00 | 0.00 | 3A4 |
| ATOM | 2926 | CG  | GLU | 411 | 12.398 | 18.662 | 1.868  | 1.00 | 0.00 | 3A4 |
| ATOM | 2927 | CD  | GLU | 411 | 12.395 | 19.342 | 0.498  | 1.00 | 0.00 | 3A4 |
| ATOM | 2928 | OE1 | GLU | 411 | 12.459 | 20.600 | 0.464  | 1.00 | 0.00 | 3A4 |
| ATOM | 2929 | OE2 | GLU | 411 | 12.316 | 18.616 | -0.530 | 1.00 | 0.00 | 3A4 |
| ATOM | 2930 | C   | GLU | 411 | 15.637 | 18.272 | 0.712  | 1.00 | 0.00 | 3A4 |
| ATOM | 2931 | O   | GLU | 411 | 15.745 | 17.227 | 0.076  | 1.00 | 0.00 | 3A4 |
| ATOM | 2932 | N   | LYS | 412 | 16.093 | 19.439 | 0.214  | 1.00 | 0.00 | 3A4 |
| ATOM | 2933 | CA  | LYS | 412 | 16.747 | 19.560 | -1.069 | 1.00 | 0.00 | 3A4 |
| ATOM | 2934 | CB  | LYS | 412 | 16.319 | 20.855 | -1.798 | 1.00 | 0.00 | 3A4 |
| ATOM | 2935 | CG  | LYS | 412 | 14.842 | 20.918 | -2.228 | 1.00 | 0.00 | 3A4 |
| ATOM | 2936 | CD  | LYS | 412 | 14.489 | 20.264 | -3.577 | 1.00 | 0.00 | 3A4 |
| ATOM | 2937 | CE  | LYS | 412 | 14.483 | 18.726 | -3.601 | 1.00 | 0.00 | 3A4 |
| ATOM | 2938 | NZ  | LYS | 412 | 13.990 | 18.220 | -4.904 | 1.00 | 0.00 | 3A4 |
| ATOM | 2939 | C   | LYS | 412 | 18.246 | 19.556 | -0.876 | 1.00 | 0.00 | 3A4 |
| ATOM | 2940 | O   | LYS | 412 | 18.788 | 20.180 | 0.031  | 1.00 | 0.00 | 3A4 |
| ATOM | 2941 | N   | PHE | 413 | 18.970 | 18.849 | -1.771 | 1.00 | 0.00 | 3A4 |
| ATOM | 2942 | CA  | PHE | 413 | 20.413 | 18.790 | -1.784 | 1.00 | 0.00 | 3A4 |
| ATOM | 2943 | CB  | PHE | 413 | 20.897 | 17.450 | -2.401 | 1.00 | 0.00 | 3A4 |
| ATOM | 2944 | CG  | PHE | 413 | 22.398 | 17.294 | -2.423 | 1.00 | 0.00 | 3A4 |
| ATOM | 2945 | CD1 | PHE | 413 | 23.168 | 17.227 | -1.254 | 1.00 | 0.00 | 3A4 |
| ATOM | 2946 | CD2 | PHE | 413 | 23.046 | 17.095 | -3.661 | 1.00 | 0.00 | 3A4 |
| ATOM | 2947 | CE1 | PHE | 413 | 24.550 | 16.999 | -1.315 | 1.00 | 0.00 | 3A4 |
| ATOM | 2948 | CE2 | PHE | 413 | 24.421 | 16.834 | -3.726 | 1.00 | 0.00 | 3A4 |
| ATOM | 2949 | CZ  | PHE | 413 | 25.177 | 16.794 | -2.550 | 1.00 | 0.00 | 3A4 |
| ATOM | 2950 | C   | PHE | 413 | 20.891 | 19.968 | -2.586 | 1.00 | 0.00 | 3A4 |
| ATOM | 2951 | O   | PHE | 413 | 20.724 | 20.009 | -3.801 | 1.00 | 0.00 | 3A4 |
| ATOM | 2952 | N   | LEU | 414 | 21.483 | 20.957 | -1.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 2953 | CA  | LEU | 414 | 21.933 | 22.177 | -2.522 | 1.00 | 0.00 | 3A4 |
| ATOM | 2954 | CB  | LEU | 414 | 20.902 | 23.301 | -2.306 | 1.00 | 0.00 | 3A4 |
| ATOM | 2955 | CG  | LEU | 414 | 21.169 | 24.700 | -2.902 | 1.00 | 0.00 | 3A4 |
| ATOM | 2956 | CD1 | LEU | 414 | 21.261 | 24.685 | -4.441 | 1.00 | 0.00 | 3A4 |
| ATOM | 2957 | CD2 | LEU | 414 | 20.079 | 25.663 | -2.388 | 1.00 | 0.00 | 3A4 |
| ATOM | 2958 | C   | LEU | 414 | 23.275 | 22.553 | -1.966 | 1.00 | 0.00 | 3A4 |
| ATOM | 2959 | O   | LEU | 414 | 23.343 | 23.031 | -0.834 | 1.00 | 0.00 | 3A4 |
| ATOM | 2960 | N   | PRO | 415 | 24.394 | 22.396 | -2.681 | 1.00 | 0.00 | 3A4 |
| ATOM | 2961 | CA  | PRO | 415 | 25.721 | 22.710 | -2.165 | 1.00 | 0.00 | 3A4 |
| ATOM | 2962 | CD  | PRO | 415 | 24.457 | 21.932 | -4.069 | 1.00 | 0.00 | 3A4 |
| ATOM | 2963 | CB  | PRO | 415 | 26.676 | 22.158 | -3.227 | 1.00 | 0.00 | 3A4 |
| ATOM | 2964 | CG  | PRO | 415 | 25.882 | 22.244 | -4.535 | 1.00 | 0.00 | 3A4 |
| ATOM | 2965 | C   | PRO | 415 | 25.978 | 24.200 | -1.983 | 1.00 | 0.00 | 3A4 |
| ATOM | 2966 | O   | PRO | 415 | 26.655 | 24.548 | -1.013 | 1.00 | 0.00 | 3A4 |
| ATOM | 2967 | N   | GLU | 416 | 25.547 | 25.077 | -2.937 | 1.00 | 0.00 | 3A4 |
| ATOM | 2968 | CA  | GLU | 416 | 25.810 | 26.505 | -2.951 | 1.00 | 0.00 | 3A4 |
| ATOM | 2969 | CB  | GLU | 416 | 27.244 | 26.943 | -3.438 | 1.00 | 0.00 | 3A4 |
| ATOM | 2970 | CG  | GLU | 416 | 28.338 | 26.841 | -2.361 | 1.00 | 0.00 | 3A4 |
| ATOM | 2971 | CD  | GLU | 416 | 29.636 | 27.541 | -2.784 | 1.00 | 0.00 | 3A4 |
| ATOM | 2972 | OE1 | GLU | 416 | 29.584 | 28.756 | -3.114 | 1.00 | 0.00 | 3A4 |
| ATOM | 2973 | OE2 | GLU | 416 | 30.704 | 26.872 | -2.759 | 1.00 | 0.00 | 3A4 |
| ATOM | 2974 | C   | GLU | 416 | 24.818 | 27.126 | -3.902 | 1.00 | 0.00 | 3A4 |
| ATOM | 2975 | O   | GLU | 416 | 24.357 | 26.500 | -4.855 | 1.00 | 0.00 | 3A4 |
| ATOM | 2976 | N   | ARG | 417 | 24.555 | 28.429 | -3.633 | 1.00 | 0.00 | 3A4 |
| ATOM | 2977 | CA  | ARG | 417 | 23.940 | 29.448 | -4.465 | 1.00 | 0.00 | 3A4 |
| ATOM | 2978 | CB  | ARG | 417 | 22.623 | 29.089 | -5.229 | 1.00 | 0.00 | 3A4 |
| ATOM | 2979 | CG  | ARG | 417 | 21.420 | 28.657 | -4.370 | 1.00 | 0.00 | 3A4 |
| ATOM | 2980 | CD  | ARG | 417 | 20.160 | 28.317 | -5.191 | 1.00 | 0.00 | 3A4 |
| ATOM | 2981 | NE  | ARG | 417 | 19.654 | 29.550 | -5.895 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 2982 | CZ  | ARG | 417 | 18.836 | 30.485 | -5.308 | 1.00 | 0.00 | 3A4 |
| ATOM | 2983 | NH1 | ARG | 417 | 18.453 | 31.575 | -6.033 | 1.00 | 0.00 | 3A4 |
| ATOM | 2984 | NH2 | ARG | 417 | 18.396 | 30.357 | -4.021 | 1.00 | 0.00 | 3A4 |
| ATOM | 2985 | C   | ARG | 417 | 23.675 | 30.614 | -3.534 | 1.00 | 0.00 | 3A4 |
| ATOM | 2986 | O   | ARG | 417 | 23.277 | 31.695 | -3.966 | 1.00 | 0.00 | 3A4 |
| ATOM | 2987 | N   | PHE | 418 | 23.883 | 30.380 | -2.207 | 1.00 | 0.00 | 3A4 |
| ATOM | 2988 | CA  | PHE | 418 | 23.598 | 31.253 | -1.087 | 1.00 | 0.00 | 3A4 |
| ATOM | 2989 | CB  | PHE | 418 | 22.842 | 30.493 | 0.064  | 1.00 | 0.00 | 3A4 |
| ATOM | 2990 | CG  | PHE | 418 | 23.400 | 29.109 | 0.354  | 1.00 | 0.00 | 3A4 |
| ATOM | 2991 | CD1 | PHE | 418 | 24.479 | 28.931 | 1.245  | 1.00 | 0.00 | 3A4 |
| ATOM | 2992 | CD2 | PHE | 418 | 22.845 | 27.967 | -0.262 | 1.00 | 0.00 | 3A4 |
| ATOM | 2993 | CE1 | PHE | 418 | 25.002 | 27.653 | 1.496  | 1.00 | 0.00 | 3A4 |
| ATOM | 2994 | CE2 | PHE | 418 | 23.361 | 26.688 | -0.007 | 1.00 | 0.00 | 3A4 |
| ATOM | 2995 | CZ  | PHE | 418 | 24.442 | 26.532 | 0.869  | 1.00 | 0.00 | 3A4 |
| ATOM | 2996 | C   | PHE | 418 | 24.891 | 31.865 | -0.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 2997 | O   | PHE | 418 | 25.978 | 31.337 | -0.822 | 1.00 | 0.00 | 3A4 |
| ATOM | 2998 | N   | SER | 419 | 24.764 | 33.010 | 0.130  | 1.00 | 0.00 | 3A4 |
| ATOM | 2999 | CA  | SER | 419 | 25.850 | 33.749 | 0.742  | 1.00 | 0.00 | 3A4 |
| ATOM | 3000 | CB  | SER | 419 | 26.168 | 35.084 | 0.003  | 1.00 | 0.00 | 3A4 |
| ATOM | 3001 | OG  | SER | 419 | 26.610 | 34.824 | -1.323 | 1.00 | 0.00 | 3A4 |
| ATOM | 3002 | C   | SER | 419 | 25.419 | 34.042 | 2.158  | 1.00 | 0.00 | 3A4 |
| ATOM | 3003 | O   | SER | 419 | 24.254 | 33.869 | 2.516  | 1.00 | 0.00 | 3A4 |
| ATOM | 3004 | N   | LYS | 420 | 26.380 | 34.507 | 2.995  | 1.00 | 0.00 | 3A4 |
| ATOM | 3005 | CA  | LYS | 420 | 26.162 | 34.853 | 4.383  | 1.00 | 0.00 | 3A4 |
| ATOM | 3006 | CB  | LYS | 420 | 26.449 | 33.660 | 5.338  | 1.00 | 0.00 | 3A4 |
| ATOM | 3007 | CG  | LYS | 420 | 26.041 | 33.882 | 6.806  | 1.00 | 0.00 | 3A4 |
| ATOM | 3008 | CD  | LYS | 420 | 25.973 | 32.611 | 7.673  | 1.00 | 0.00 | 3A4 |
| ATOM | 3009 | CE  | LYS | 420 | 27.316 | 31.947 | 8.025  | 1.00 | 0.00 | 3A4 |
| ATOM | 3010 | NZ  | LYS | 420 | 27.897 | 31.201 | 6.884  | 1.00 | 0.00 | 3A4 |
| ATOM | 3011 | C   | LYS | 420 | 27.070 | 36.024 | 4.656  | 1.00 | 0.00 | 3A4 |
| ATOM | 3012 | O   | LYS | 420 | 28.205 | 36.070 | 4.182  | 1.00 | 0.00 | 3A4 |
| ATOM | 3013 | N   | LYS | 421 | 26.554 | 37.018 | 5.432  | 1.00 | 0.00 | 3A4 |
| ATOM | 3014 | CA  | LYS | 421 | 27.150 | 38.319 | 5.697  | 1.00 | 0.00 | 3A4 |
| ATOM | 3015 | CB  | LYS | 421 | 26.041 | 39.410 | 5.739  | 1.00 | 0.00 | 3A4 |
| ATOM | 3016 | CG  | LYS | 421 | 26.518 | 40.872 | 5.751  | 1.00 | 0.00 | 3A4 |
| ATOM | 3017 | CD  | LYS | 421 | 25.360 | 41.868 | 5.629  | 1.00 | 0.00 | 3A4 |
| ATOM | 3018 | CE  | LYS | 421 | 25.821 | 43.332 | 5.619  | 1.00 | 0.00 | 3A4 |
| ATOM | 3019 | NZ  | LYS | 421 | 24.664 | 44.251 | 5.492  | 1.00 | 0.00 | 3A4 |
| ATOM | 3020 | C   | LYS | 421 | 27.940 | 38.313 | 6.992  | 1.00 | 0.00 | 3A4 |
| ATOM | 3021 | O   | LYS | 421 | 28.871 | 39.099 | 7.165  | 1.00 | 0.00 | 3A4 |
| ATOM | 3022 | N   | ASN | 422 | 27.572 | 37.398 | 7.933  | 1.00 | 0.00 | 3A4 |
| ATOM | 3023 | CA  | ASN | 422 | 28.154 | 37.237 | 9.255  | 1.00 | 0.00 | 3A4 |
| ATOM | 3024 | CB  | ASN | 422 | 27.020 | 37.047 | 10.319 | 1.00 | 0.00 | 3A4 |
| ATOM | 3025 | CG  | ASN | 422 | 27.499 | 37.210 | 11.776 | 1.00 | 0.00 | 3A4 |
| ATOM | 3026 | OD1 | ASN | 422 | 27.456 | 36.260 | 12.556 | 1.00 | 0.00 | 3A4 |
| ATOM | 3027 | ND2 | ASN | 422 | 27.964 | 38.434 | 12.149 | 1.00 | 0.00 | 3A4 |
| ATOM | 3028 | C   | ASN | 422 | 29.107 | 36.052 | 9.222  | 1.00 | 0.00 | 3A4 |
| ATOM | 3029 | O   | ASN | 422 | 29.035 | 35.203 | 8.335  | 1.00 | 0.00 | 3A4 |
| ATOM | 3030 | N   | LYS | 423 | 30.033 | 35.989 | 10.220 | 1.00 | 0.00 | 3A4 |
| ATOM | 3031 | CA  | LYS | 423 | 31.052 | 34.968 | 10.382 | 1.00 | 0.00 | 3A4 |
| ATOM | 3032 | CB  | LYS | 423 | 32.450 | 35.576 | 10.704 | 1.00 | 0.00 | 3A4 |
| ATOM | 3033 | CG  | LYS | 423 | 33.030 | 36.450 | 9.575  | 1.00 | 0.00 | 3A4 |
| ATOM | 3034 | CD  | LYS | 423 | 33.266 | 35.769 | 8.209  | 1.00 | 0.00 | 3A4 |
| ATOM | 3035 | CE  | LYS | 423 | 34.431 | 34.762 | 8.142  | 1.00 | 0.00 | 3A4 |
| ATOM | 3036 | NZ  | LYS | 423 | 34.107 | 33.470 | 8.794  | 1.00 | 0.00 | 3A4 |
| ATOM | 3037 | C   | LYS | 423 | 30.631 | 34.032 | 11.491 | 1.00 | 0.00 | 3A4 |
| ATOM | 3038 | O   | LYS | 423 | 30.939 | 34.245 | 12.663 | 1.00 | 0.00 | 3A4 |
| ATOM | 3039 | N   | ASP | 424 | 29.907 | 32.953 | 11.101 | 1.00 | 0.00 | 3A4 |
| ATOM | 3040 | CA  | ASP | 424 | 29.457 | 31.893 | 11.976 | 1.00 | 0.00 | 3A4 |
| ATOM | 3041 | CB  | ASP | 424 | 28.060 | 32.147 | 12.651 | 1.00 | 0.00 | 3A4 |
| ATOM | 3042 | CG  | ASP | 424 | 26.909 | 32.519 | 11.687 | 1.00 | 0.00 | 3A4 |
| ATOM | 3043 | OD1 | ASP | 424 | 25.944 | 31.714 | 11.589 | 1.00 | 0.00 | 3A4 |
| ATOM | 3044 | OD2 | ASP | 424 | 26.973 | 33.604 | 11.051 | 1.00 | 0.00 | 3A4 |
| ATOM | 3045 | C   | ASP | 424 | 29.495 | 30.648 | 11.123 | 1.00 | 0.00 | 3A4 |
| ATOM | 3046 | O   | ASP | 424 | 28.470 | 30.043 | 10.811 | 1.00 | 0.00 | 3A4 |
| ATOM | 3047 | N   | ASN | 425 | 30.728 | 30.251 | 10.724 | 1.00 | 0.00 | 3A4 |
| ATOM | 3048 | CA  | ASN | 425 | 30.999 | 29.112 | 9.872  | 1.00 | 0.00 | 3A4 |
| ATOM | 3049 | CB  | ASN | 425 | 30.910 | 29.449 | 8.339  | 1.00 | 0.00 | 3A4 |
| ATOM | 3050 | CG  | ASN | 425 | 31.718 | 30.701 | 7.912  | 1.00 | 0.00 | 3A4 |
| ATOM | 3051 | OD1 | ASN | 425 | 32.894 | 30.588 | 7.570  | 1.00 | 0.00 | 3A4 |
| ATOM | 3052 | ND2 | ASN | 425 | 31.085 | 31.907 | 7.916  | 1.00 | 0.00 | 3A4 |
| ATOM | 3053 | C   | ASN | 425 | 32.363 | 28.587 | 10.270 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 3054 | O   | ASN | 425 | 33.092 | 28.033 | 9.449  | 1.00 | 0.00 | 3A4 |
| ATOM | 3055 | N   | ILE | 426 | 32.734 | 28.773 | 11.570 | 1.00 | 0.00 | 3A4 |
| ATOM | 3056 | CA  | ILE | 426 | 34.043 | 28.493 | 12.137 | 1.00 | 0.00 | 3A4 |
| ATOM | 3057 | CB  | ILE | 426 | 34.648 | 29.716 | 12.854 | 1.00 | 0.00 | 3A4 |
| ATOM | 3058 | CG2 | ILE | 426 | 36.105 | 29.402 | 13.297 | 1.00 | 0.00 | 3A4 |
| ATOM | 3059 | CG1 | ILE | 426 | 34.591 | 30.966 | 11.928 | 1.00 | 0.00 | 3A4 |
| ATOM | 3060 | CD  | ILE | 426 | 35.100 | 32.260 | 12.569 | 1.00 | 0.00 | 3A4 |
| ATOM | 3061 | C   | ILE | 426 | 33.870 | 27.289 | 13.047 | 1.00 | 0.00 | 3A4 |
| ATOM | 3062 | O   | ILE | 426 | 34.107 | 26.155 | 12.633 | 1.00 | 0.00 | 3A4 |
| ATOM | 3063 | N   | ASP | 427 | 33.447 | 27.532 | 14.315 | 1.00 | 0.00 | 3A4 |
| ATOM | 3064 | CA  | ASP | 427 | 33.204 | 26.537 | 15.348 | 1.00 | 0.00 | 3A4 |
| ATOM | 3065 | CB  | ASP | 427 | 34.320 | 26.450 | 16.444 | 1.00 | 0.00 | 3A4 |
| ATOM | 3066 | CG  | ASP | 427 | 35.639 | 25.963 | 15.828 | 1.00 | 0.00 | 3A4 |
| ATOM | 3067 | OD1 | ASP | 427 | 35.660 | 24.821 | 15.293 | 1.00 | 0.00 | 3A4 |
| ATOM | 3068 | OD2 | ASP | 427 | 36.643 | 26.722 | 15.888 | 1.00 | 0.00 | 3A4 |
| ATOM | 3069 | C   | ASP | 427 | 31.841 | 26.813 | 15.973 | 1.00 | 0.00 | 3A4 |
| ATOM | 3070 | O   | ASP | 427 | 31.098 | 25.842 | 16.103 | 1.00 | 0.00 | 3A4 |
| ATOM | 3071 | N   | PRO | 428 | 31.390 | 28.043 | 16.369 | 1.00 | 0.00 | 3A4 |
| ATOM | 3072 | CA  | PRO | 428 | 29.983 | 28.361 | 16.637 | 1.00 | 0.00 | 3A4 |
| ATOM | 3073 | CD  | PRO | 428 | 32.272 | 29.141 | 16.778 | 1.00 | 0.00 | 3A4 |
| ATOM | 3074 | CB  | PRO | 428 | 30.041 | 29.613 | 17.539 | 1.00 | 0.00 | 3A4 |
| ATOM | 3075 | CG  | PRO | 428 | 31.359 | 30.308 | 17.172 | 1.00 | 0.00 | 3A4 |
| ATOM | 3076 | C   | PRO | 428 | 29.245 | 28.611 | 15.321 | 1.00 | 0.00 | 3A4 |
| ATOM | 3077 | O   | PRO | 428 | 29.471 | 29.640 | 14.687 | 1.00 | 0.00 | 3A4 |
| ATOM | 3078 | N   | TYR | 429 | 28.385 | 27.650 | 14.899 | 1.00 | 0.00 | 3A4 |
| ATOM | 3079 | CA  | TYR | 429 | 27.755 | 27.649 | 13.596 | 1.00 | 0.00 | 3A4 |
| ATOM | 3080 | CB  | TYR | 429 | 28.727 | 27.191 | 12.437 | 1.00 | 0.00 | 3A4 |
| ATOM | 3081 | CG  | TYR | 429 | 29.325 | 25.786 | 12.428 | 1.00 | 0.00 | 3A4 |
| ATOM | 3082 | CD1 | TYR | 429 | 29.871 | 25.334 | 11.208 | 1.00 | 0.00 | 3A4 |
| ATOM | 3083 | CD2 | TYR | 429 | 29.371 | 24.901 | 13.532 | 1.00 | 0.00 | 3A4 |
| ATOM | 3084 | CE1 | TYR | 429 | 30.418 | 24.050 | 11.078 | 1.00 | 0.00 | 3A4 |
| ATOM | 3085 | CE2 | TYR | 429 | 29.917 | 23.615 | 13.410 | 1.00 | 0.00 | 3A4 |
| ATOM | 3086 | CZ  | TYR | 429 | 30.437 | 23.186 | 12.181 | 1.00 | 0.00 | 3A4 |
| ATOM | 3087 | OH  | TYR | 429 | 30.972 | 21.885 | 12.055 | 1.00 | 0.00 | 3A4 |
| ATOM | 3088 | C   | TYR | 429 | 26.500 | 26.805 | 13.683 | 1.00 | 0.00 | 3A4 |
| ATOM | 3089 | O   | TYR | 429 | 25.984 | 26.542 | 14.769 | 1.00 | 0.00 | 3A4 |
| ATOM | 3090 | N   | ILE | 430 | 26.004 | 26.339 | 12.499 | 1.00 | 0.00 | 3A4 |
| ATOM | 3091 | CA  | ILE | 430 | 24.912 | 25.392 | 12.301 | 1.00 | 0.00 | 3A4 |
| ATOM | 3092 | CB  | ILE | 430 | 23.953 | 25.845 | 11.196 | 1.00 | 0.00 | 3A4 |
| ATOM | 3093 | CG2 | ILE | 430 | 23.323 | 27.171 | 11.680 | 1.00 | 0.00 | 3A4 |
| ATOM | 3094 | CG1 | ILE | 430 | 24.623 | 26.004 | 9.800  | 1.00 | 0.00 | 3A4 |
| ATOM | 3095 | CD  | ILE | 430 | 23.667 | 26.472 | 8.700  | 1.00 | 0.00 | 3A4 |
| ATOM | 3096 | C   | ILE | 430 | 25.562 | 24.051 | 12.005 | 1.00 | 0.00 | 3A4 |
| ATOM | 3097 | O   | ILE | 430 | 26.789 | 23.977 | 12.016 | 1.00 | 0.00 | 3A4 |
| ATOM | 3098 | N   | TYR | 431 | 24.773 | 22.951 | 11.760 | 1.00 | 0.00 | 3A4 |
| ATOM | 3099 | CA  | TYR | 431 | 25.198 | 21.604 | 11.414 | 1.00 | 0.00 | 3A4 |
| ATOM | 3100 | CB  | TYR | 431 | 26.437 | 21.470 | 10.410 | 1.00 | 0.00 | 3A4 |
| ATOM | 3101 | CG  | TYR | 431 | 26.384 | 22.218 | 9.097  | 1.00 | 0.00 | 3A4 |
| ATOM | 3102 | CD1 | TYR | 431 | 25.749 | 21.647 | 7.983  | 1.00 | 0.00 | 3A4 |
| ATOM | 3103 | CD2 | TYR | 431 | 27.142 | 23.393 | 8.894  | 1.00 | 0.00 | 3A4 |
| ATOM | 3104 | CE1 | TYR | 431 | 25.834 | 22.246 | 6.714  | 1.00 | 0.00 | 3A4 |
| ATOM | 3105 | CE2 | TYR | 431 | 27.212 | 24.010 | 7.638  | 1.00 | 0.00 | 3A4 |
| ATOM | 3106 | CZ  | TYR | 431 | 26.551 | 23.437 | 6.544  | 1.00 | 0.00 | 3A4 |
| ATOM | 3107 | OH  | TYR | 431 | 26.632 | 24.036 | 5.267  | 1.00 | 0.00 | 3A4 |
| ATOM | 3108 | C   | TYR | 431 | 25.647 | 20.889 | 12.688 | 1.00 | 0.00 | 3A4 |
| ATOM | 3109 | O   | TYR | 431 | 26.635 | 21.285 | 13.303 | 1.00 | 0.00 | 3A4 |
| ATOM | 3110 | N   | THR | 432 | 24.989 | 19.782 | 13.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 3111 | CA  | THR | 432 | 25.445 | 18.960 | 14.203 | 1.00 | 0.00 | 3A4 |
| ATOM | 3112 | CB  | THR | 432 | 24.381 | 18.938 | 15.316 | 1.00 | 0.00 | 3A4 |
| ATOM | 3113 | OG1 | THR | 432 | 23.070 | 18.659 | 14.826 | 1.00 | 0.00 | 3A4 |
| ATOM | 3114 | CG2 | THR | 432 | 24.399 | 20.310 | 16.028 | 1.00 | 0.00 | 3A4 |
| ATOM | 3115 | C   | THR | 432 | 25.810 | 17.558 | 13.781 | 1.00 | 0.00 | 3A4 |
| ATOM | 3116 | O   | THR | 432 | 25.565 | 16.648 | 14.576 | 1.00 | 0.00 | 3A4 |
| ATOM | 3117 | N   | PRO | 433 | 26.389 | 17.234 | 12.610 | 1.00 | 0.00 | 3A4 |
| ATOM | 3118 | CA  | PRO | 433 | 26.601 | 15.849 | 12.240 | 1.00 | 0.00 | 3A4 |
| ATOM | 3119 | CD  | PRO | 433 | 27.173 | 18.101 | 11.724 | 1.00 | 0.00 | 3A4 |
| ATOM | 3120 | CB  | PRO | 433 | 26.947 | 15.918 | 10.740 | 1.00 | 0.00 | 3A4 |
| ATOM | 3121 | CG  | PRO | 433 | 27.743 | 17.221 | 10.601 | 1.00 | 0.00 | 3A4 |
| ATOM | 3122 | C   | PRO | 433 | 27.748 | 15.209 | 13.022 | 1.00 | 0.00 | 3A4 |
| ATOM | 3123 | O   | PRO | 433 | 27.771 | 13.993 | 13.150 | 1.00 | 0.00 | 3A4 |
| ATOM | 3124 | N   | PHE | 434 | 28.673 | 16.013 | 13.587 | 1.00 | 0.00 | 3A4 |
| ATOM | 3125 | CA  | PHE | 434 | 29.782 | 15.548 | 14.382 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |         |        |        |      |      |     |
|------|------|-----|-----|-----|---------|--------|--------|------|------|-----|
| ATOM | 3126 | CB  | PHE | 434 | 31.108  | 16.257 | 13.997 | 1.00 | 0.00 | 3A4 |
| ATOM | 3127 | CG  | PHE | 434 | 31.591  | 15.810 | 12.639 | 1.00 | 0.00 | 3A4 |
| ATOM | 3128 | CD1 | PHE | 434 | 31.353  | 16.451 | 11.514 | 1.00 | 0.00 | 3A4 |
| ATOM | 3129 | CD2 | PHE | 434 | 32.354  | 14.754 | 12.363 | 1.00 | 0.00 | 3A4 |
| ATOM | 3130 | CE1 | PHE | 434 | 31.813  | 16.203 | 10.200 | 1.00 | 0.00 | 3A4 |
| ATOM | 3131 | CE2 | PHE | 434 | 32.860  | 14.287 | 11.129 | 1.00 | 0.00 | 3A4 |
| ATOM | 3132 | CZ  | PHE | 434 | 32.592  | 15.066 | 10.009 | 1.00 | 0.00 | 3A4 |
| ATOM | 3133 | C   | PHE | 434 | 29.528  | 15.802 | 15.833 | 1.00 | 0.00 | 3A4 |
| ATOM | 3134 | O   | PHE | 434 | 30.427  | 15.663 | 16.655 | 1.00 | 0.00 | 3A4 |
| ATOM | 3135 | N   | GLY | 435 | 28.291  | 16.210 | 16.191 | 1.00 | 0.00 | 3A4 |
| ATOM | 3136 | CA  | GLY | 435 | 27.923  | 16.495 | 17.561 | 1.00 | 0.00 | 3A4 |
| ATOM | 3137 | C   | GLY | 435 | 28.209  | 17.917 | 17.875 | 1.00 | 0.00 | 3A4 |
| ATOM | 3138 | O   | GLY | 435 | 28.305  | 18.719 | 16.943 | 1.00 | 0.00 | 3A4 |
| ATOM | 3139 | N   | SER | 436 | 28.348  | 18.248 | 19.183 | 1.00 | 0.00 | 3A4 |
| ATOM | 3140 | CA  | SER | 436 | 28.384  | 19.623 | 19.578 | 1.00 | 0.00 | 3A4 |
| ATOM | 3141 | CB  | SER | 436 | 26.947  | 20.258 | 19.543 | 1.00 | 0.00 | 3A4 |
| ATOM | 3142 | OG  | SER | 436 | 26.948  | 21.683 | 19.489 | 1.00 | 0.00 | 3A4 |
| ATOM | 3143 | C   | SER | 436 | 29.197  | 19.916 | 20.769 | 1.00 | 0.00 | 3A4 |
| ATOM | 3144 | O   | SER | 436 | 30.134  | 20.642 | 20.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 3145 | N   | GLY | 437 | 28.951  | 19.486 | 21.973 | 1.00 | 0.00 | 3A4 |
| ATOM | 3146 | CA  | GLY | 437 | 29.675  | 19.961 | 23.144 | 1.00 | 0.00 | 3A4 |
| ATOM | 3147 | C   | GLY | 437 | 31.130  | 19.558 | 23.314 | 1.00 | 0.00 | 3A4 |
| ATOM | 3148 | O   | GLY | 437 | 31.959  | 19.487 | 22.402 | 1.00 | 0.00 | 3A4 |
| ATOM | 3149 | N   | PRO | 438 | 31.502  | 19.228 | 24.529 | 1.00 | 0.00 | 3A4 |
| ATOM | 3150 | CA  | PRO | 438 | 32.875  | 18.727 | 24.776 | 1.00 | 0.00 | 3A4 |
| ATOM | 3151 | CD  | PRO | 438 | 30.927  | 19.742 | 25.770 | 1.00 | 0.00 | 3A4 |
| ATOM | 3152 | CB  | PRO | 438 | 33.100  | 18.880 | 26.266 | 1.00 | 0.00 | 3A4 |
| ATOM | 3153 | CG  | PRO | 438 | 31.706  | 19.063 | 26.880 | 1.00 | 0.00 | 3A4 |
| ATOM | 3154 | C   | PRO | 438 | 33.099  | 17.295 | 24.317 | 1.00 | 0.00 | 3A4 |
| ATOM | 3155 | O   | PRO | 438 | 34.230  | 16.824 | 24.348 | 1.00 | 0.00 | 3A4 |
| ATOM | 3156 | N   | ARG | 439 | 32.033  | 16.608 | 23.850 | 1.00 | 0.00 | 3A4 |
| ATOM | 3157 | CA  | ARG | 439 | 32.068  | 15.264 | 23.366 | 1.00 | 0.00 | 3A4 |
| ATOM | 3158 | CB  | ARG | 439 | 30.905  | 14.467 | 23.961 | 1.00 | 0.00 | 3A4 |
| ATOM | 3159 | CG  | ARG | 439 | 30.793  | 14.766 | 25.461 | 1.00 | 0.00 | 3A4 |
| ATOM | 3160 | CD  | ARG | 439 | 30.197  | 13.690 | 26.366 | 1.00 | 0.00 | 3A4 |
| ATOM | 3161 | NE  | ARG | 439 | 30.391  | 14.136 | 27.786 | 1.00 | 0.00 | 3A4 |
| ATOM | 3162 | CZ  | ARG | 439 | 30.091  | 13.354 | 28.866 | 1.00 | 0.00 | 3A4 |
| ATOM | 3163 | NH1 | ARG | 439 | 30.342  | 13.836 | 30.116 | 1.00 | 0.00 | 3A4 |
| ATOM | 3164 | NH2 | ARG | 439 | 29.553  | 12.109 | 28.713 | 1.00 | 0.00 | 3A4 |
| ATOM | 3165 | C   | ARG | 439 | 31.980  | 15.221 | 21.890 | 1.00 | 0.00 | 3A4 |
| ATOM | 3166 | O   | ARG | 439 | 31.776  | 14.165 | 21.309 | 1.00 | 0.00 | 3A4 |
| ATOM | 3167 | N   | ASN | 440 | 32.201  | 16.364 | 21.200 | 1.00 | 0.00 | 3A4 |
| ATOM | 3168 | CA  | ASN | 440 | 32.204  | 16.474 | 19.756 | 1.00 | 0.00 | 3A4 |
| ATOM | 3169 | CB  | ASN | 440 | 32.625  | 17.886 | 19.354 | 1.00 | 0.00 | 3A4 |
| ATOM | 3170 | CG  | ASN | 440 | 32.279  | 18.329 | 17.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 3171 | OD1 | ASN | 440 | 32.746  | 17.778 | 16.907 | 1.00 | 0.00 | 3A4 |
| ATOM | 3172 | ND2 | ASN | 440 | 31.452  | 19.401 | 17.765 | 1.00 | 0.00 | 3A4 |
| ATOM | 3173 | C   | ASN | 440 | 33.216  | 15.539 | 19.171 | 1.00 | 0.00 | 3A4 |
| ATOM | 3174 | O   | ASN | 440 | 34.241  | 15.285 | 19.807 | 1.00 | 0.00 | 3A4 |
| ATOM | 3175 | N   | CYS | 441 | 32.950  | 14.993 | 17.974 | 1.00 | 0.00 | 3A4 |
| ATOM | 3176 | CA  | CYS | 441 | 33.782  | 14.009 | 17.328 | 1.00 | 0.00 | 3A4 |
| ATOM | 3177 | CB  | CYS | 441 | 33.288  | 13.772 | 15.899 | 1.00 | 0.00 | 3A4 |
| ATOM | 3178 | SG  | CYS | 441 | 34.028  | 12.338 | 15.029 | 1.00 | 0.00 | 3A4 |
| ATOM | 3179 | C   | CYS | 441 | 35.241  | 14.414 | 17.264 | 1.00 | 0.00 | 3A4 |
| ATOM | 3180 | O   | CYS | 441 | 35.564  | 15.528 | 16.866 | 1.00 | 0.00 | 3A4 |
| ATOM | 3181 | N   | ILE | 442 | -36.131 | 13.531 | 17.746 | 1.00 | 0.00 | 3A4 |
| ATOM | 3182 | CA  | ILE | 442 | 37.556  | 13.799 | 17.790 | 1.00 | 0.00 | 3A4 |
| ATOM | 3183 | CB  | ILE | 442 | 38.223  | 12.944 | 18.848 | 1.00 | 0.00 | 3A4 |
| ATOM | 3184 | CG2 | ILE | 442 | 38.388  | 11.476 | 18.448 | 1.00 | 0.00 | 3A4 |
| ATOM | 3185 | CG1 | ILE | 442 | 39.528  | 13.570 | 19.391 | 1.00 | 0.00 | 3A4 |
| ATOM | 3186 | CD  | ILE | 442 | 39.336  | 14.819 | 20.250 | 1.00 | 0.00 | 3A4 |
| ATOM | 3187 | C   | ILE | 442 | 38.181  | 13.605 | 16.408 | 1.00 | 0.00 | 3A4 |
| ATOM | 3188 | O   | ILE | 442 | 39.180  | 14.220 | 16.048 | 1.00 | 0.00 | 3A4 |
| ATOM | 3189 | N   | GLY | 443 | 37.524  | 12.758 | 15.590 | 1.00 | 0.00 | 3A4 |
| ATOM | 3190 | CA  | GLY | 443 | 37.942  | 12.408 | 14.266 | 1.00 | 0.00 | 3A4 |
| ATOM | 3191 | C   | GLY | 443 | 37.399  | 13.252 | 13.158 | 1.00 | 0.00 | 3A4 |
| ATOM | 3192 | O   | GLY | 443 | 37.591  | 12.902 | 12.001 | 1.00 | 0.00 | 3A4 |
| ATOM | 3193 | N   | MET | 444 | 36.732  | 14.396 | 13.456 | 1.00 | 0.00 | 3A4 |
| ATOM | 3194 | CA  | MET | 444 | 36.082  | 15.266 | 12.493 | 1.00 | 0.00 | 3A4 |
| ATOM | 3195 | CB  | MET | 444 | 35.408  | 16.458 | 13.192 | 1.00 | 0.00 | 3A4 |
| ATOM | 3196 | CG  | MET | 444 | 36.294  | 17.310 | 14.126 | 1.00 | 0.00 | 3A4 |
| ATOM | 3197 | SD  | MET | 444 | 35.375  | 18.583 | 15.041 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 3198 | CE  | MET | 444 | 36.695 | 18.911 | 16.244 | 1.00 | 0.00 | 3A4 |
| ATOM | 3199 | C   | MET | 444 | 36.968 | 15.807 | 11.395 | 1.00 | 0.00 | 3A4 |
| ATOM | 3200 | O   | MET | 444 | 36.570 | 15.844 | 10.236 | 1.00 | 0.00 | 3A4 |
| ATOM | 3201 | N   | ARG | 445 | 38.230 | 16.170 | 11.727 | 1.00 | 0.00 | 3A4 |
| ATOM | 3202 | CA  | ARG | 445 | 39.211 | 16.708 | 10.801 | 1.00 | 0.00 | 3A4 |
| ATOM | 3203 | CB  | ARG | 445 | 40.435 | 17.321 | 11.549 | 1.00 | 0.00 | 3A4 |
| ATOM | 3204 | CG  | ARG | 445 | 40.058 | 18.332 | 12.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 3205 | CD  | ARG | 445 | 39.223 | 19.529 | 12.155 | 1.00 | 0.00 | 3A4 |
| ATOM | 3206 | NE  | ARG | 445 | 38.880 | 20.389 | 13.341 | 1.00 | 0.00 | 3A4 |
| ATOM | 3207 | CZ  | ARG | 445 | 37.901 | 21.351 | 13.313 | 1.00 | 0.00 | 3A4 |
| ATOM | 3208 | NH1 | ARG | 445 | 37.643 | 22.071 | 14.443 | 1.00 | 0.00 | 3A4 |
| ATOM | 3209 | NH2 | ARG | 445 | 37.171 | 21.600 | 12.186 | 1.00 | 0.00 | 3A4 |
| ATOM | 3210 | C   | ARG | 445 | 39.695 | 15.651 | 9.828  | 1.00 | 0.00 | 3A4 |
| ATOM | 3211 | O   | ARG | 445 | 39.790 | 15.886 | 8.628  | 1.00 | 0.00 | 3A4 |
| ATOM | 3212 | N   | PHE | 446 | 39.920 | 14.418 | 10.335 | 1.00 | 0.00 | 3A4 |
| ATOM | 3213 | CA  | PHE | 446 | 40.293 | 13.256 | 9.549  | 1.00 | 0.00 | 3A4 |
| ATOM | 3214 | CB  | PHE | 446 | 40.683 | 12.116 | 10.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 3215 | CG  | PHE | 446 | 41.549 | 11.008 | 9.982  | 1.00 | 0.00 | 3A4 |
| ATOM | 3216 | CD1 | PHE | 446 | 42.800 | 11.292 | 9.403  | 1.00 | 0.00 | 3A4 |
| ATOM | 3217 | CD2 | PHE | 446 | 41.248 | 9.684  | 10.350 | 1.00 | 0.00 | 3A4 |
| ATOM | 3218 | CE1 | PHE | 446 | 43.749 | 10.278 | 9.241  | 1.00 | 0.00 | 3A4 |
| ATOM | 3219 | CE2 | PHE | 446 | 42.210 | 8.678  | 10.222 | 1.00 | 0.00 | 3A4 |
| ATOM | 3220 | CZ  | PHE | 446 | 43.469 | 8.983  | 9.689  | 1.00 | 0.00 | 3A4 |
| ATOM | 3221 | C   | PHE | 446 | 39.172 | 12.804 | 8.647  | 1.00 | 0.00 | 3A4 |
| ATOM | 3222 | O   | PHE | 446 | 39.384 | 12.508 | 7.480  | 1.00 | 0.00 | 3A4 |
| ATOM | 3223 | N   | ALA | 447 | 37.921 | 12.812 | 9.148  | 1.00 | 0.00 | 3A4 |
| ATOM | 3224 | CA  | ALA | 447 | 36.738 | 12.472 | 8.393  | 1.00 | 0.00 | 3A4 |
| ATOM | 3225 | CB  | ALA | 447 | 35.499 | 12.464 | 9.272  | 1.00 | 0.00 | 3A4 |
| ATOM | 3226 | C   | ALA | 447 | 36.489 | 13.392 | 7.228  | 1.00 | 0.00 | 3A4 |
| ATOM | 3227 | O   | ALA | 447 | 36.216 | 12.950 | 6.120  | 1.00 | 0.00 | 3A4 |
| ATOM | 3228 | N   | LEU | 448 | 36.656 | 14.715 | 7.427  | 1.00 | 0.00 | 3A4 |
| ATOM | 3229 | CA  | LEU | 448 | 36.469 | 15.704 | 6.386  | 1.00 | 0.00 | 3A4 |
| ATOM | 3230 | CB  | LEU | 448 | 36.399 | 17.124 | 6.962  | 1.00 | 0.00 | 3A4 |
| ATOM | 3231 | CG  | LEU | 448 | 35.089 | 17.408 | 7.731  | 1.00 | 0.00 | 3A4 |
| ATOM | 3232 | CD1 | LEU | 448 | 35.223 | 18.721 | 8.515  | 1.00 | 0.00 | 3A4 |
| ATOM | 3233 | CD2 | LEU | 448 | 33.842 | 17.445 | 6.826  | 1.00 | 0.00 | 3A4 |
| ATOM | 3234 | C   | LEU | 448 | 37.561 | 15.661 | 5.351  | 1.00 | 0.00 | 3A4 |
| ATOM | 3235 | O   | LEU | 448 | 37.299 | 15.865 | 4.175  | 1.00 | 0.00 | 3A4 |
| ATOM | 3236 | N   | MET | 449 | 38.806 | 15.319 | 5.746  | 1.00 | 0.00 | 3A4 |
| ATOM | 3237 | CA  | MET | 449 | 39.935 | 15.178 | 4.853  | 1.00 | 0.00 | 3A4 |
| ATOM | 3238 | CB  | MET | 449 | 41.269 | 15.033 | 5.617  | 1.00 | 0.00 | 3A4 |
| ATOM | 3239 | CG  | MET | 449 | 41.841 | 16.358 | 6.130  | 1.00 | 0.00 | 3A4 |
| ATOM | 3240 | SD  | MET | 449 | 43.382 | 16.135 | 7.075  | 1.00 | 0.00 | 3A4 |
| ATOM | 3241 | CE  | MET | 449 | 43.701 | 17.904 | 7.332  | 1.00 | 0.00 | 3A4 |
| ATOM | 3242 | C   | MET | 449 | 39.772 | 13.984 | 3.951  | 1.00 | 0.00 | 3A4 |
| ATOM | 3243 | O   | MET | 449 | 39.956 | 14.095 | 2.746  | 1.00 | 0.00 | 3A4 |
| ATOM | 3244 | N   | ASN | 450 | 39.332 | 12.829 | 4.502  | 1.00 | 0.00 | 3A4 |
| ATOM | 3245 | CA  | ASN | 450 | 39.098 | 11.625 | 3.740  | 1.00 | 0.00 | 3A4 |
| ATOM | 3246 | CB  | ASN | 450 | 38.915 | 10.385 | 4.623  | 1.00 | 0.00 | 3A4 |
| ATOM | 3247 | CG  | ASN | 450 | 37.685 | 10.130 | 5.531  | 1.00 | 0.00 | 3A4 |
| ATOM | 3248 | OD1 | ASN | 450 | 36.512 | 10.268 | 5.191  | 1.00 | 0.00 | 3A4 |
| ATOM | 3249 | ND2 | ASN | 450 | 37.990 | 9.606  | 6.751  | 1.00 | 0.00 | 3A4 |
| ATOM | 3250 | C   | ASN | 450 | 37.976 | 11.740 | 2.750  | 1.00 | 0.00 | 3A4 |
| ATOM | 3251 | O   | ASN | 450 | 38.095 | 11.281 | 1.623  | 1.00 | 0.00 | 3A4 |
| ATOM | 3252 | N   | MET | 451 | 36.874 | 12.422 | 3.129  | 1.00 | 0.00 | 3A4 |
| ATOM | 3253 | CA  | MET | 451 | 35.744 | 12.687 | 2.267  | 1.00 | 0.00 | 3A4 |
| ATOM | 3254 | CB  | MET | 451 | 34.596 | 13.445 | 3.021  | 1.00 | 0.00 | 3A4 |
| ATOM | 3255 | CG  | MET | 451 | 33.788 | 12.610 | 4.010  | 1.00 | 0.00 | 3A4 |
| ATOM | 3256 | SD  | MET | 451 | 32.502 | 13.565 | 4.863  | 1.00 | 0.00 | 3A4 |
| ATOM | 3257 | CE  | MET | 451 | 33.061 | 13.383 | 6.570  | 1.00 | 0.00 | 3A4 |
| ATOM | 3258 | C   | MET | 451 | 36.081 | 13.580 | 1.106  | 1.00 | 0.00 | 3A4 |
| ATOM | 3259 | O   | MET | 451 | 35.746 | 13.314 | -0.041 | 1.00 | 0.00 | 3A4 |
| ATOM | 3260 | N   | LYS | 452 | 36.821 | 14.667 | 1.389  | 1.00 | 0.00 | 3A4 |
| ATOM | 3261 | CA  | LYS | 452 | 37.237 | 15.652 | 0.424  | 1.00 | 0.00 | 3A4 |
| ATOM | 3262 | CB  | LYS | 452 | 37.854 | 16.860 | 1.154  | 1.00 | 0.00 | 3A4 |
| ATOM | 3263 | CG  | LYS | 452 | 37.750 | 18.227 | 0.470  | 1.00 | 0.00 | 3A4 |
| ATOM | 3264 | CD  | LYS | 452 | 38.346 | 19.380 | 1.301  | 1.00 | 0.00 | 3A4 |
| ATOM | 3265 | CE  | LYS | 452 | 38.006 | 19.391 | 2.808  | 1.00 | 0.00 | 3A4 |
| ATOM | 3266 | NZ  | LYS | 452 | 36.543 | 19.337 | 3.053  | 1.00 | 0.00 | 3A4 |
| ATOM | 3267 | C   | LYS | 452 | 38.228 | 15.110 | -0.572 | 1.00 | 0.00 | 3A4 |
| ATOM | 3268 | O   | LYS | 452 | 38.108 | 15.335 | -1.769 | 1.00 | 0.00 | 3A4 |
| ATOM | 3269 | N   | LEU | 453 | 39.207 | 14.309 | -0.102 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 3270 | CA  | LEU | 453 | 40.212 | 13.676 | -0.927  | 1.00 | 0.00 | 3A4 |
| ATOM | 3271 | CB  | LEU | 453 | 41.342 | 13.071 | -0.061  | 1.00 | 0.00 | 3A4 |
| ATOM | 3272 | CG  | LEU | 453 | 42.298 | 14.219 | 0.403   | 1.00 | 0.00 | 3A4 |
| ATOM | 3273 | CD1 | LEU | 453 | 43.187 | 13.854 | 1.595   | 1.00 | 0.00 | 3A4 |
| ATOM | 3274 | CD2 | LEU | 453 | 43.191 | 14.764 | -0.734  | 1.00 | 0.00 | 3A4 |
| ATOM | 3275 | C   | LEU | 453 | 39.621 | 12.644 | -1.845  | 1.00 | 0.00 | 3A4 |
| ATOM | 3276 | O   | LEU | 453 | 39.939 | 12.613 | -3.026  | 1.00 | 0.00 | 3A4 |
| ATOM | 3277 | N   | ALA | 454 | 38.662 | 11.829 | -1.353  | 1.00 | 0.00 | 3A4 |
| ATOM | 3278 | CA  | ALA | 454 | 37.935 | 10.847 | -2.131  | 1.00 | 0.00 | 3A4 |
| ATOM | 3279 | CB  | ALA | 454 | 37.013 | 9.992  | -1.240  | 1.00 | 0.00 | 3A4 |
| ATOM | 3280 | C   | ALA | 454 | 37.093 | 11.464 | -3.225  | 1.00 | 0.00 | 3A4 |
| ATOM | 3281 | O   | ALA | 454 | 37.181 | 11.055 | -4.371  | 1.00 | 0.00 | 3A4 |
| ATOM | 3282 | N   | LEU | 455 | 36.307 | 12.514 | -2.904  | 1.00 | 0.00 | 3A4 |
| ATOM | 3283 | CA  | LEU | 455 | 35.457 | 13.201 | -3.852  | 1.00 | 0.00 | 3A4 |
| ATOM | 3284 | CB  | LEU | 455 | 34.480 | 14.157 | -3.157  | 1.00 | 0.00 | 3A4 |
| ATOM | 3285 | CG  | LEU | 455 | 33.366 | 13.559 | -2.303  | 1.00 | 0.00 | 3A4 |
| ATOM | 3286 | CD1 | LEU | 455 | 32.576 | 14.761 | -1.760  | 1.00 | 0.00 | 3A4 |
| ATOM | 3287 | CD2 | LEU | 455 | 32.474 | 12.556 | -3.064  | 1.00 | 0.00 | 3A4 |
| ATOM | 3288 | C   | LEU | 455 | 36.203 | 14.018 | -4.886  | 1.00 | 0.00 | 3A4 |
| ATOM | 3289 | O   | LEU | 455 | 35.736 | 14.147 | -6.009  | 1.00 | 0.00 | 3A4 |
| ATOM | 3290 | N   | ILE | 456 | 37.412 | 14.540 | -4.555  | 1.00 | 0.00 | 3A4 |
| ATOM | 3291 | CA  | ILE | 456 | 38.284 | 15.264 | -5.474  | 1.00 | 0.00 | 3A4 |
| ATOM | 3292 | CB  | ILE | 456 | 39.413 | 16.061 | -4.749  | 1.00 | 0.00 | 3A4 |
| ATOM | 3293 | CG2 | ILE | 456 | 40.832 | 16.074 | -5.412  | 1.00 | 0.00 | 3A4 |
| ATOM | 3294 | CG1 | ILE | 456 | 39.003 | 17.537 | -4.565  | 1.00 | 0.00 | 3A4 |
| ATOM | 3295 | CD  | ILE | 456 | 38.041 | 17.823 | -3.423  | 1.00 | 0.00 | 3A4 |
| ATOM | 3296 | C   | ILE | 456 | 38.894 | 14.318 | -6.496  | 1.00 | 0.00 | 3A4 |
| ATOM | 3297 | O   | ILE | 456 | 39.099 | 14.677 | -7.647  | 1.00 | 0.00 | 3A4 |
| ATOM | 3298 | N   | ARG | 457 | 39.181 | 13.066 | -6.083  | 1.00 | 0.00 | 3A4 |
| ATOM | 3299 | CA  | ARG | 457 | 39.859 | 12.081 | -6.895  | 1.00 | 0.00 | 3A4 |
| ATOM | 3300 | CB  | ARG | 457 | 40.758 | 11.186 | -6.025  | 1.00 | 0.00 | 3A4 |
| ATOM | 3301 | CG  | ARG | 457 | 41.905 | 12.005 | -5.430  | 1.00 | 0.00 | 3A4 |
| ATOM | 3302 | CD  | ARG | 457 | 42.735 | 11.300 | -4.341  | 1.00 | 0.00 | 3A4 |
| ATOM | 3303 | NE  | ARG | 457 | 43.559 | 12.343 | -3.632  | 1.00 | 0.00 | 3A4 |
| ATOM | 3304 | CZ  | ARG | 457 | 44.624 | 12.985 | -4.211  | 1.00 | 0.00 | 3A4 |
| ATOM | 3305 | NH1 | ARG | 457 | 45.148 | 14.087 | -3.601  | 1.00 | 0.00 | 3A4 |
| ATOM | 3306 | NH2 | ARG | 457 | 45.174 | 12.558 | -5.385  | 1.00 | 0.00 | 3A4 |
| ATOM | 3307 | C   | ARG | 457 | 38.924 | 11.235 | -7.722  | 1.00 | 0.00 | 3A4 |
| ATOM | 3308 | O   | ARG | 457 | 39.246 | 10.873 | -8.848  | 1.00 | 0.00 | 3A4 |
| ATOM | 3309 | N   | VAL | 458 | 37.713 | 10.918 | -7.207  | 1.00 | 0.00 | 3A4 |
| ATOM | 3310 | CA  | VAL | 458 | 36.711 | 10.092 | -7.872  | 1.00 | 0.00 | 3A4 |
| ATOM | 3311 | CB  | VAL | 458 | 35.631 | 9.662  | -6.887  | 1.00 | 0.00 | 3A4 |
| ATOM | 3312 | CG1 | VAL | 458 | 34.290 | 9.133  | -7.471  | 1.00 | 0.00 | 3A4 |
| ATOM | 3313 | CG2 | VAL | 458 | 36.253 | 8.556  | -6.006  | 1.00 | 0.00 | 3A4 |
| ATOM | 3314 | C   | VAL | 458 | 36.101 | 10.798 | -9.063  | 1.00 | 0.00 | 3A4 |
| ATOM | 3315 | O   | VAL | 458 | 36.040 | 10.236 | -10.146 | 1.00 | 0.00 | 3A4 |
| ATOM | 3316 | N   | LEU | 459 | 35.685 | 12.071 | -8.900  | 1.00 | 0.00 | 3A4 |
| ATOM | 3317 | CA  | LEU | 459 | 34.979 | 12.841 | -9.906  | 1.00 | 0.00 | 3A4 |
| ATOM | 3318 | CB  | LEU | 459 | 34.354 | 14.096 | -9.255  | 1.00 | 0.00 | 3A4 |
| ATOM | 3319 | CG  | LEU | 459 | 33.225 | 13.778 | -8.265  | 1.00 | 0.00 | 3A4 |
| ATOM | 3320 | CD1 | LEU | 459 | 32.786 | 15.037 | -7.500  | 1.00 | 0.00 | 3A4 |
| ATOM | 3321 | CD2 | LEU | 459 | 32.041 | 13.132 | -8.991  | 1.00 | 0.00 | 3A4 |
| ATOM | 3322 | C   | LEU | 459 | 35.826 | 13.309 | -11.060 | 1.00 | 0.00 | 3A4 |
| ATOM | 3323 | O   | LEU | 459 | 35.319 | 13.601 | -12.136 | 1.00 | 0.00 | 3A4 |
| ATOM | 3324 | N   | GLN | 460 | 37.158 | 13.371 | -10.874 | 1.00 | 0.00 | 3A4 |
| ATOM | 3325 | CA  | GLN | 460 | 38.070 | 13.748 | -11.927 | 1.00 | 0.00 | 3A4 |
| ATOM | 3326 | CB  | GLN | 460 | 39.373 | 14.365 | -11.376 | 1.00 | 0.00 | 3A4 |
| ATOM | 3327 | CG  | GLN | 460 | 39.106 | 15.740 | -10.736 | 1.00 | 0.00 | 3A4 |
| ATOM | 3328 | CD  | GLN | 460 | 40.408 | 16.286 | -10.160 | 1.00 | 0.00 | 3A4 |
| ATOM | 3329 | OE1 | GLN | 460 | 41.430 | 15.608 | -10.237 | 1.00 | 0.00 | 3A4 |
| ATOM | 3330 | NE2 | GLN | 460 | 40.380 | 17.515 | -9.575  | 1.00 | 0.00 | 3A4 |
| ATOM | 3331 | C   | GLN | 460 | 38.365 | 12.562 | -12.815 | 1.00 | 0.00 | 3A4 |
| ATOM | 3332 | O   | GLN | 460 | 38.683 | 12.730 | -13.990 | 1.00 | 0.00 | 3A4 |
| ATOM | 3333 | N   | ASN | 461 | 38.258 | 11.332 | -12.266 | 1.00 | 0.00 | 3A4 |
| ATOM | 3334 | CA  | ASN | 461 | 38.598 | 10.113 | -12.957 | 1.00 | 0.00 | 3A4 |
| ATOM | 3335 | CB  | ASN | 461 | 39.328 | 9.125  | -12.018 | 1.00 | 0.00 | 3A4 |
| ATOM | 3336 | CG  | ASN | 461 | 40.725 | 9.722  | -11.730 | 1.00 | 0.00 | 3A4 |
| ATOM | 3337 | OD1 | ASN | 461 | 41.364 | 10.283 | -12.617 | 1.00 | 0.00 | 3A4 |
| ATOM | 3338 | ND2 | ASN | 461 | 41.239 | 9.604  | -10.482 | 1.00 | 0.00 | 3A4 |
| ATOM | 3339 | C   | ASN | 461 | 37.402 | 9.427  | -13.562 | 1.00 | 0.00 | 3A4 |
| ATOM | 3340 | O   | ASN | 461 | 37.588 | 8.603  | -14.451 | 1.00 | 0.00 | 3A4 |
| ATOM | 3341 | N   | PHE | 462 | 36.167 | 9.725  | -13.107 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 3342 | CA  | PHE | 462 | 34.983 | 8.975  | -13.533 | 1.00 | 0.00 | 3A4 |
| ATOM | 3343 | CB  | PHE | 462 | 34.346 | 8.159  | -12.354 | 1.00 | 0.00 | 3A4 |
| ATOM | 3344 | CG  | PHE | 462 | 35.274 | 7.073  | -11.873 | 1.00 | 0.00 | 3A4 |
| ATOM | 3345 | CD1 | PHE | 462 | 35.686 | 6.051  | -12.745 | 1.00 | 0.00 | 3A4 |
| ATOM | 3346 | CD2 | PHE | 462 | 35.718 | 7.025  | -10.540 | 1.00 | 0.00 | 3A4 |
| ATOM | 3347 | CE1 | PHE | 462 | 36.530 | 5.021  | -12.307 | 1.00 | 0.00 | 3A4 |
| ATOM | 3348 | CE2 | PHE | 462 | 36.561 | 6.001  | -10.089 | 1.00 | 0.00 | 3A4 |
| ATOM | 3349 | CZ  | PHE | 462 | 36.972 | 5.002  | -10.978 | 1.00 | 0.00 | 3A4 |
| ATOM | 3350 | C   | PHE | 462 | 33.836 | 9.848  | -14.135 | 1.00 | 0.00 | 3A4 |
| ATOM | 3351 | O   | PHE | 462 | 33.734 | 11.037 | -13.828 | 1.00 | 0.00 | 3A4 |
| ATOM | 3352 | N   | SER | 463 | 32.784 | 9.198  | -15.007 | 1.00 | 0.00 | 3A4 |
| ATOM | 3353 | CA  | SER | 463 | 31.446 | 9.622  | -15.542 | 1.00 | 0.00 | 3A4 |
| ATOM | 3354 | CB  | SER | 463 | 31.400 | 9.685  | -17.094 | 1.00 | 0.00 | 3A4 |
| ATOM | 3355 | OG  | SER | 463 | 32.293 | 10.684 | -17.565 | 1.00 | 0.00 | 3A4 |
| ATOM | 3356 | C   | SER | 463 | 30.513 | 8.581  | -15.014 | 1.00 | 0.00 | 3A4 |
| ATOM | 3357 | O   | SER | 463 | 30.243 | 7.578  | -15.673 | 1.00 | 0.00 | 3A4 |
| ATOM | 3358 | N   | PHE | 464 | 30.012 | 8.774  | -13.767 | 1.00 | 0.00 | 3A4 |
| ATOM | 3359 | CA  | PHE | 464 | 29.251 | 7.754  | -13.078 | 1.00 | 0.00 | 3A4 |
| ATOM | 3360 | CB  | PHE | 464 | 29.689 | 7.483  | -11.603 | 1.00 | 0.00 | 3A4 |
| ATOM | 3361 | CG  | PHE | 464 | 29.600 | 8.582  | -10.565 | 1.00 | 0.00 | 3A4 |
| ATOM | 3362 | CD1 | PHE | 464 | 30.780 | 9.102  | -9.999  | 1.00 | 0.00 | 3A4 |
| ATOM | 3363 | CD2 | PHE | 464 | 28.364 | 8.952  | -9.990  | 1.00 | 0.00 | 3A4 |
| ATOM | 3364 | CE1 | PHE | 464 | 30.727 | 9.958  | -8.891  | 1.00 | 0.00 | 3A4 |
| ATOM | 3365 | CE2 | PHE | 464 | 28.310 | 9.832  | -8.899  | 1.00 | 0.00 | 3A4 |
| ATOM | 3366 | CZ  | PHE | 464 | 29.493 | 10.333 | -8.347  | 1.00 | 0.00 | 3A4 |
| ATOM | 3367 | C   | PHE | 464 | 27.768 | 7.948  | -13.199 | 1.00 | 0.00 | 3A4 |
| ATOM | 3368 | O   | PHE | 464 | 27.238 | 9.056  | -13.175 | 1.00 | 0.00 | 3A4 |
| ATOM | 3369 | N   | LYS | 465 | 27.076 | 6.801  | -13.331 | 1.00 | 0.00 | 3A4 |
| ATOM | 3370 | CA  | LYS | 465 | 25.646 | 6.719  | -13.439 | 1.00 | 0.00 | 3A4 |
| ATOM | 3371 | CB  | LYS | 465 | 25.197 | 6.398  | -14.891 | 1.00 | 0.00 | 3A4 |
| ATOM | 3372 | CG  | LYS | 465 | 25.553 | 7.484  | -15.915 | 1.00 | 0.00 | 3A4 |
| ATOM | 3373 | CD  | LYS | 465 | 25.067 | 7.162  | -17.333 | 1.00 | 0.00 | 3A4 |
| ATOM | 3374 | CE  | LYS | 465 | 25.438 | 8.228  | -18.374 | 1.00 | 0.00 | 3A4 |
| ATOM | 3375 | NZ  | LYS | 465 | 26.910 | 8.360  | -18.512 | 1.00 | 0.00 | 3A4 |
| ATOM | 3376 | C   | LYS | 465 | 25.212 | 5.614  | -12.507 | 1.00 | 0.00 | 3A4 |
| ATOM | 3377 | O   | LYS | 465 | 25.982 | 4.688  | -12.254 | 1.00 | 0.00 | 3A4 |
| ATOM | 3378 | N   | PRO | 466 | 23.983 | 5.622  | -11.985 | 1.00 | 0.00 | 3A4 |
| ATOM | 3379 | CA  | PRO | 466 | 23.422 | 4.511  | -11.249 | 1.00 | 0.00 | 3A4 |
| ATOM | 3380 | CD  | PRO | 466 | 23.090 | 6.783  | -11.993 | 1.00 | 0.00 | 3A4 |
| ATOM | 3381 | CB  | PRO | 466 | 22.300 | 5.151  | -10.405 | 1.00 | 0.00 | 3A4 |
| ATOM | 3382 | CG  | PRO | 466 | 21.827 | 6.358  | -11.228 | 1.00 | 0.00 | 3A4 |
| ATOM | 3383 | C   | PRO | 466 | 22.906 | 3.470  | -12.228 | 1.00 | 0.00 | 3A4 |
| ATOM | 3384 | O   | PRO | 466 | 22.333 | 3.808  | -13.264 | 1.00 | 0.00 | 3A4 |
| ATOM | 3385 | N   | CYS | 467 | 23.088 | 2.179  | -11.890 | 1.00 | 0.00 | 3A4 |
| ATOM | 3386 | CA  | CYS | 467 | 22.624 | 1.049  | -12.667 | 1.00 | 0.00 | 3A4 |
| ATOM | 3387 | CB  | CYS | 467 | 23.617 | -0.143 | -12.501 | 1.00 | 0.00 | 3A4 |
| ATOM | 3388 | SG  | CYS | 467 | 23.434 | -1.534 | -13.674 | 1.00 | 0.00 | 3A4 |
| ATOM | 3389 | C   | CYS | 467 | 21.212 | 0.659  | -12.220 | 1.00 | 0.00 | 3A4 |
| ATOM | 3390 | O   | CYS | 467 | 20.555 | -0.179 | -12.834 | 1.00 | 0.00 | 3A4 |
| ATOM | 3391 | N   | LYS | 468 | 20.726 | 1.325  | -11.130 | 1.00 | 0.00 | 3A4 |
| ATOM | 3392 | CA  | LYS | 468 | 19.389 | 1.282  | -10.573 | 1.00 | 0.00 | 3A4 |
| ATOM | 3393 | CB  | LYS | 468 | 19.406 | 1.410  | -9.027  | 1.00 | 0.00 | 3A4 |
| ATOM | 3394 | CG  | LYS | 468 | 20.290 | 0.367  | -8.339  | 1.00 | 0.00 | 3A4 |
| ATOM | 3395 | CD  | LYS | 468 | 20.136 | 0.413  | -6.821  | 1.00 | 0.00 | 3A4 |
| ATOM | 3396 | CE  | LYS | 468 | 21.077 | -0.534 | -6.078  | 1.00 | 0.00 | 3A4 |
| ATOM | 3397 | NZ  | LYS | 468 | 20.807 | -0.485 | -4.626  | 1.00 | 0.00 | 3A4 |
| ATOM | 3398 | C   | LYS | 468 | 18.586 | 2.429  | -11.148 | 1.00 | 0.00 | 3A4 |
| ATOM | 3399 | O   | LYS | 468 | 19.145 | 3.450  | -11.548 | 1.00 | 0.00 | 3A4 |
| ATOM | 3400 | N   | GLU | 469 | 17.238 | 2.263  | -11.203 | 1.00 | 0.00 | 3A4 |
| ATOM | 3401 | CA  | GLU | 469 | 16.301 | 3.177  | -11.832 | 1.00 | 0.00 | 3A4 |
| ATOM | 3402 | CB  | GLU | 469 | 15.428 | 2.446  | -12.905 | 1.00 | 0.00 | 3A4 |
| ATOM | 3403 | CG  | GLU | 469 | 16.234 | 1.719  | -14.000 | 1.00 | 0.00 | 3A4 |
| ATOM | 3404 | CD  | GLU | 469 | 17.104 | 2.712  | -14.780 | 1.00 | 0.00 | 3A4 |
| ATOM | 3405 | OE1 | GLU | 469 | 16.530 | 3.642  | -15.407 | 1.00 | 0.00 | 3A4 |
| ATOM | 3406 | OE2 | GLU | 469 | 18.355 | 2.551  | -14.761 | 1.00 | 0.00 | 3A4 |
| ATOM | 3407 | C   | GLU | 469 | 15.433 | 3.792  | -10.753 | 1.00 | 0.00 | 3A4 |
| ATOM | 3408 | O   | GLU | 469 | 15.841 | 3.909  | -9.598  | 1.00 | 0.00 | 3A4 |
| ATOM | 3409 | N   | THR | 470 | 14.183 | 4.182  | -11.133 | 1.00 | 0.00 | 3A4 |
| ATOM | 3410 | CA  | THR | 470 | 13.125 | 4.722  | -10.289 | 1.00 | 0.00 | 3A4 |
| ATOM | 3411 | CB  | THR | 470 | 12.400 | 5.877  | -10.998 | 1.00 | 0.00 | 3A4 |
| ATOM | 3412 | OG1 | THR | 470 | 11.519 | 6.597  | -10.138 | 1.00 | 0.00 | 3A4 |
| ATOM | 3413 | CG2 | THR | 470 | 11.657 | 5.427  | -12.286 | 1.00 | 0.00 | 3A4 |



|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 3414 | C   | THR | 470 | 12.198 | 3.578  | -9.882  | 1.00 | 0.00 | 3A4 |
| ATOM | 3415 | O   | THR | 470 | 11.456 | 3.677  | -8.906  | 1.00 | 0.00 | 3A4 |
| ATOM | 3416 | N   | GLN | 471 | 12.279 | 2.447  | -10.640 | 1.00 | 0.00 | 3A4 |
| ATOM | 3417 | CA  | GLN | 471 | 11.670 | 1.158  | -10.385 | 1.00 | 0.00 | 3A4 |
| ATOM | 3418 | CB  | GLN | 471 | 10.997 | 0.559  | -11.656 | 1.00 | 0.00 | 3A4 |
| ATOM | 3419 | CG  | GLN | 471 | 11.811 | 0.665  | -12.967 | 1.00 | 0.00 | 3A4 |
| ATOM | 3420 | CD  | GLN | 471 | 10.976 | 0.103  | -14.119 | 1.00 | 0.00 | 3A4 |
| ATOM | 3421 | OE1 | GLN | 471 | 10.763 | -1.106 | -14.193 | 1.00 | 0.00 | 3A4 |
| ATOM | 3422 | NE2 | GLN | 471 | 10.489 | 0.985  | -15.035 | 1.00 | 0.00 | 3A4 |
| ATOM | 3423 | C   | GLN | 471 | 12.773 | 0.276  | -9.839  | 1.00 | 0.00 | 3A4 |
| ATOM | 3424 | O   | GLN | 471 | 13.605 | -0.249 | -10.577 | 1.00 | 0.00 | 3A4 |
| ATOM | 3425 | N   | ILE | 472 | 12.809 | 0.178  | -8.475  | 1.00 | 0.00 | 3A4 |
| ATOM | 3426 | CA  | ILE | 472 | 13.847 | -0.369 | -7.600  | 1.00 | 0.00 | 3A4 |
| ATOM | 3427 | CB  | ILE | 472 | 14.451 | -1.737 | -7.993  | 1.00 | 0.00 | 3A4 |
| ATOM | 3428 | CG2 | ILE | 472 | 15.447 | -2.232 | -6.907  | 1.00 | 0.00 | 3A4 |
| ATOM | 3429 | CG1 | ILE | 472 | 13.359 | -2.820 | -8.240  | 1.00 | 0.00 | 3A4 |
| ATOM | 3430 | CD  | ILE | 472 | 12.440 | -3.129 | -7.050  | 1.00 | 0.00 | 3A4 |
| ATOM | 3431 | C   | ILE | 472 | 14.926 | 0.710  | -7.400  | 1.00 | 0.00 | 3A4 |
| ATOM | 3432 | O   | ILE | 472 | 15.870 | 0.760  | -8.188  | 1.00 | 0.00 | 3A4 |
| ATOM | 3433 | N   | PRO | 473 | 14.837 | 1.594  | -6.373  | 1.00 | 0.00 | 3A4 |
| ATOM | 3434 | CA  | PRO | 473 | 15.865 | 2.553  | -5.978  | 1.00 | 0.00 | 3A4 |
| ATOM | 3435 | CD  | PRO | 473 | 13.607 | 1.778  | -5.600  | 1.00 | 0.00 | 3A4 |
| ATOM | 3436 | CB  | PRO | 473 | 15.047 | 3.657  | -5.263  | 1.00 | 0.00 | 3A4 |
| ATOM | 3437 | CG  | PRO | 473 | 13.885 | 2.910  | -4.607  | 1.00 | 0.00 | 3A4 |
| ATOM | 3438 | C   | PRO | 473 | 16.926 | 1.936  | -5.117  | 1.00 | 0.00 | 3A4 |
| ATOM | 3439 | O   | PRO | 473 | 17.147 | 0.726  | -5.098  | 1.00 | 0.00 | 3A4 |
| ATOM | 3440 | N   | LEU | 474 | 17.606 | 2.821  | -4.384  | 1.00 | 0.00 | 3A4 |
| ATOM | 3441 | CA  | LEU | 474 | 18.692 | 2.518  | -3.506  | 1.00 | 0.00 | 3A4 |
| ATOM | 3442 | CB  | LEU | 474 | 19.658 | 3.718  | -3.467  | 1.00 | 0.00 | 3A4 |
| ATOM | 3443 | CG  | LEU | 474 | 20.935 | 3.548  | -2.623  | 1.00 | 0.00 | 3A4 |
| ATOM | 3444 | CD1 | LEU | 474 | 22.187 | 3.637  | -3.503  | 1.00 | 0.00 | 3A4 |
| ATOM | 3445 | CD2 | LEU | 474 | 20.962 | 4.569  | -1.472  | 1.00 | 0.00 | 3A4 |
| ATOM | 3446 | C   | LEU | 474 | 18.157 | 2.198  | -2.136  | 1.00 | 0.00 | 3A4 |
| ATOM | 3447 | O   | LEU | 474 | 17.397 | 2.966  | -1.547  | 1.00 | 0.00 | 3A4 |
| ATOM | 3448 | N   | LYS | 475 | 18.561 | 1.016  | -1.612  | 1.00 | 0.00 | 3A4 |
| ATOM | 3449 | CA  | LYS | 475 | 18.133 | 0.502  | -0.330  | 1.00 | 0.00 | 3A4 |
| ATOM | 3450 | CB  | LYS | 475 | 18.199 | -1.049 | -0.249  | 1.00 | 0.00 | 3A4 |
| ATOM | 3451 | CG  | LYS | 475 | 17.520 | -1.656 | 0.999   | 1.00 | 0.00 | 3A4 |
| ATOM | 3452 | CD  | LYS | 475 | 17.579 | -3.189 | 1.074   | 1.00 | 0.00 | 3A4 |
| ATOM | 3453 | CE  | LYS | 475 | 18.981 | -3.776 | 1.311   | 1.00 | 0.00 | 3A4 |
| ATOM | 3454 | NZ  | LYS | 475 | 19.572 | -3.282 | 2.580   | 1.00 | 0.00 | 3A4 |
| ATOM | 3455 | C   | LYS | 475 | 18.961 | 1.086  | 0.775   | 1.00 | 0.00 | 3A4 |
| ATOM | 3456 | O   | LYS | 475 | 20.173 | 0.909  | 0.825   | 1.00 | 0.00 | 3A4 |
| ATOM | 3457 | N   | LEU | 476 | 18.276 | 1.798  | 1.695   | 1.00 | 0.00 | 3A4 |
| ATOM | 3458 | CA  | LEU | 476 | 18.860 | 2.419  | 2.855   | 1.00 | 0.00 | 3A4 |
| ATOM | 3459 | CB  | LEU | 476 | 18.422 | 3.903  | 3.070   | 1.00 | 0.00 | 3A4 |
| ATOM | 3460 | CG  | LEU | 476 | 16.930 | 4.243  | 3.360   | 1.00 | 0.00 | 3A4 |
| ATOM | 3461 | CD1 | LEU | 476 | 16.813 | 5.725  | 3.764   | 1.00 | 0.00 | 3A4 |
| ATOM | 3462 | CD2 | LEU | 476 | 15.956 | 3.930  | 2.201   | 1.00 | 0.00 | 3A4 |
| ATOM | 3463 | C   | LEU | 476 | 18.580 | 1.579  | 4.038   | 1.00 | 0.00 | 3A4 |
| ATOM | 3464 | O   | LEU | 476 | 17.524 | 0.970  | 4.149   | 1.00 | 0.00 | 3A4 |
| ATOM | 3465 | N   | SER | 477 | 19.543 | 1.495  | 4.973   | 1.00 | 0.00 | 3A4 |
| ATOM | 3466 | CA  | SER | 477 | 19.480 | 0.545  | 6.040   | 1.00 | 0.00 | 3A4 |
| ATOM | 3467 | CB  | SER | 477 | 20.807 | -0.220 | 6.343   | 1.00 | 0.00 | 3A4 |
| ATOM | 3468 | OG  | SER | 477 | 20.584 | -1.554 | 6.795   | 1.00 | 0.00 | 3A4 |
| ATOM | 3469 | C   | SER | 477 | 18.826 | 1.150  | 7.228   | 1.00 | 0.00 | 3A4 |
| ATOM | 3470 | O   | SER | 477 | 18.936 | 2.334  | 7.525   | 1.00 | 0.00 | 3A4 |
| ATOM | 3471 | N   | LEU | 478 | 18.068 | 0.282  | 7.917   | 1.00 | 0.00 | 3A4 |
| ATOM | 3472 | CA  | LEU | 478 | 17.386 | 0.588  | 9.132   | 1.00 | 0.00 | 3A4 |
| ATOM | 3473 | CB  | LEU | 478 | 16.072 | -0.245 | 9.288   | 1.00 | 0.00 | 3A4 |
| ATOM | 3474 | CG  | LEU | 478 | 15.314 | -0.208 | 10.653  | 1.00 | 0.00 | 3A4 |
| ATOM | 3475 | CD1 | LEU | 478 | 14.954 | 1.206  | 11.152  | 1.00 | 0.00 | 3A4 |
| ATOM | 3476 | CD2 | LEU | 478 | 14.057 | -1.098 | 10.607  | 1.00 | 0.00 | 3A4 |
| ATOM | 3477 | C   | LEU | 478 | 18.338 | 0.280  | 10.281  | 1.00 | 0.00 | 3A4 |
| ATOM | 3478 | O   | LEU | 478 | 18.566 | -0.855 | 10.665  | 1.00 | 0.00 | 3A4 |
| ATOM | 3479 | N   | GLY | 479 | 18.982 | 1.308  | 10.841  | 1.00 | 0.00 | 3A4 |
| ATOM | 3480 | CA  | GLY | 479 | 19.983 | 1.119  | 11.875  | 1.00 | 0.00 | 3A4 |
| ATOM | 3481 | C   | GLY | 479 | 19.558 | 1.665  | 13.192  | 1.00 | 0.00 | 3A4 |
| ATOM | 3482 | O   | GLY | 479 | 19.405 | 0.936  | 14.154  | 1.00 | 0.00 | 3A4 |
| ATOM | 3483 | N   | GLY | 480 | 19.416 | 2.996  | 13.329  | 1.00 | 0.00 | 3A4 |
| ATOM | 3484 | CA  | GLY | 480 | 19.205 | 3.607  | 14.623  | 1.00 | 0.00 | 3A4 |
| ATOM | 3485 | C   | GLY | 480 | 20.442 | 4.355  | 14.943  | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 3486 | O   | GLY | 480 | 20.430 | 5.574  | 14.961 | 1.00 | 0.00 | 3A4 |
| ATOM | 3487 | N   | LEU | 481 | 21.566 | 3.643  | 15.196 | 1.00 | 0.00 | 3A4 |
| ATOM | 3488 | CA  | LEU | 481 | 22.833 | 4.218  | 15.597 | 1.00 | 0.00 | 3A4 |
| ATOM | 3489 | CB  | LEU | 481 | 23.634 | 3.303  | 16.586 | 1.00 | 0.00 | 3A4 |
| ATOM | 3490 | CG  | LEU | 481 | 23.971 | 1.830  | 16.194 | 1.00 | 0.00 | 3A4 |
| ATOM | 3491 | CD1 | LEU | 481 | 25.057 | 1.273  | 17.135 | 1.00 | 0.00 | 3A4 |
| ATOM | 3492 | CD2 | LEU | 481 | 22.767 | 0.861  | 16.168 | 1.00 | 0.00 | 3A4 |
| ATOM | 3493 | C   | LEU | 481 | 23.664 | 4.637  | 14.398 | 1.00 | 0.00 | 3A4 |
| ATOM | 3494 | O   | LEU | 481 | 24.121 | 5.774  | 14.349 | 1.00 | 0.00 | 3A4 |
| ATOM | 3495 | N   | LEU | 482 | 23.838 | 3.733  | 13.398 | 1.00 | 0.00 | 3A4 |
| ATOM | 3496 | CA  | LEU | 482 | 24.486 | 3.984  | 12.124 | 1.00 | 0.00 | 3A4 |
| ATOM | 3497 | CB  | LEU | 482 | 25.613 | 2.951  | 11.765 | 1.00 | 0.00 | 3A4 |
| ATOM | 3498 | CG  | LEU | 482 | 26.965 | 3.067  | 12.517 | 1.00 | 0.00 | 3A4 |
| ATOM | 3499 | CD1 | LEU | 482 | 27.722 | 4.365  | 12.213 | 1.00 | 0.00 | 3A4 |
| ATOM | 3500 | CD2 | LEU | 482 | 26.897 | 2.808  | 14.028 | 1.00 | 0.00 | 3A4 |
| ATOM | 3501 | C   | LEU | 482 | 23.378 | 3.835  | 11.115 | 1.00 | 0.00 | 3A4 |
| ATOM | 3502 | O   | LEU | 482 | 22.784 | 2.766  | 11.044 | 1.00 | 0.00 | 3A4 |
| ATOM | 3503 | N   | GLN | 483 | 23.090 | 4.887  | 10.291 | 1.00 | 0.00 | 3A4 |
| ATOM | 3504 | CA  | GLN | 483 | 22.131 | 4.849  | 9.194  | 1.00 | 0.00 | 3A4 |
| ATOM | 3505 | CB  | GLN | 483 | 21.199 | 6.105  | 9.194  | 1.00 | 0.00 | 3A4 |
| ATOM | 3506 | CG  | GLN | 483 | 20.316 | 6.274  | 10.449 | 1.00 | 0.00 | 3A4 |
| ATOM | 3507 | CD  | GLN | 483 | 19.134 | 5.295  | 10.458 | 1.00 | 0.00 | 3A4 |
| ATOM | 3508 | OE1 | GLN | 483 | 18.982 | 4.423  | 9.605  | 1.00 | 0.00 | 3A4 |
| ATOM | 3509 | NE2 | GLN | 483 | 18.236 | 5.459  | 11.467 | 1.00 | 0.00 | 3A4 |
| ATOM | 3510 | C   | GLN | 483 | 22.916 | 4.815  | 7.900  | 1.00 | 0.00 | 3A4 |
| ATOM | 3511 | O   | GLN | 483 | 23.541 | 5.820  | 7.606  | 1.00 | 0.00 | 3A4 |
| ATOM | 3512 | N   | PRO | 484 | 22.951 | 3.748  | 7.093  | 1.00 | 0.00 | 3A4 |
| ATOM | 3513 | CA  | PRO | 484 | 23.817 | 3.721  | 5.925  | 1.00 | 0.00 | 3A4 |
| ATOM | 3514 | CD  | PRO | 484 | 22.874 | 2.409  | 7.687  | 1.00 | 0.00 | 3A4 |
| ATOM | 3515 | CB  | PRO | 484 | 24.769 | 2.558  | 6.262  | 1.00 | 0.00 | 3A4 |
| ATOM | 3516 | CG  | PRO | 484 | 23.861 | 1.520  | 6.915  | 1.00 | 0.00 | 3A4 |
| ATOM | 3517 | C   | PRO | 484 | 23.035 | 3.412  | 4.673  | 1.00 | 0.00 | 3A4 |
| ATOM | 3518 | O   | PRO | 484 | 21.816 | 3.307  | 4.680  | 1.00 | 0.00 | 3A4 |
| ATOM | 3519 | N   | GLU | 485 | 23.773 | 3.212  | 3.562  | 1.00 | 0.00 | 3A4 |
| ATOM | 3520 | CA  | GLU | 485 | 23.248 | 2.558  | 2.383  | 1.00 | 0.00 | 3A4 |
| ATOM | 3521 | CB  | GLU | 485 | 23.098 | 3.493  | 1.177  | 1.00 | 0.00 | 3A4 |
| ATOM | 3522 | CG  | GLU | 485 | 24.327 | 4.316  | 0.781  | 1.00 | 0.00 | 3A4 |
| ATOM | 3523 | CD  | GLU | 485 | 24.829 | 3.771  | -0.540 | 1.00 | 0.00 | 3A4 |
| ATOM | 3524 | OE1 | GLU | 485 | 24.837 | 4.541  | -1.536 | 1.00 | 0.00 | 3A4 |
| ATOM | 3525 | OE2 | GLU | 485 | 25.209 | 2.571  | -0.567 | 1.00 | 0.00 | 3A4 |
| ATOM | 3526 | C   | GLU | 485 | 24.043 | 1.288  | 2.206  | 1.00 | 0.00 | 3A4 |
| ATOM | 3527 | O   | GLU | 485 | 25.260 | 1.289  | 2.296  | 1.00 | 0.00 | 3A4 |
| ATOM | 3528 | N   | LYS | 486 | 23.368 | 0.126  | 2.027  | 1.00 | 0.00 | 3A4 |
| ATOM | 3529 | CA  | LYS | 486 | 24.038 | -1.172 | 1.973  | 1.00 | 0.00 | 3A4 |
| ATOM | 3530 | CB  | LYS | 486 | 23.286 | -2.272 | 2.791  | 1.00 | 0.00 | 3A4 |
| ATOM | 3531 | CG  | LYS | 486 | 24.070 | -3.558 | 3.141  | 1.00 | 0.00 | 3A4 |
| ATOM | 3532 | CD  | LYS | 486 | 24.136 | -4.672 | 2.074  | 1.00 | 0.00 | 3A4 |
| ATOM | 3533 | CE  | LYS | 486 | 22.782 | -5.249 | 1.626  | 1.00 | 0.00 | 3A4 |
| ATOM | 3534 | NZ  | LYS | 486 | 22.037 | -5.839 | 2.765  | 1.00 | 0.00 | 3A4 |
| ATOM | 3535 | C   | LYS | 486 | 24.427 | -1.507 | 0.545  | 1.00 | 0.00 | 3A4 |
| ATOM | 3536 | O   | LYS | 486 | 25.595 | -1.841 | 0.334  | 1.00 | 0.00 | 3A4 |
| ATOM | 3537 | N   | PRO | 487 | 23.564 | -1.396 | -0.475 | 1.00 | 0.00 | 3A4 |
| ATOM | 3538 | CA  | PRO | 487 | 23.980 | -1.646 | -1.846 | 1.00 | 0.00 | 3A4 |
| ATOM | 3539 | CD  | PRO | 487 | 22.127 | -1.666 | -0.334 | 1.00 | 0.00 | 3A4 |
| ATOM | 3540 | CB  | PRO | 487 | 22.967 | -2.687 | -2.354 | 1.00 | 0.00 | 3A4 |
| ATOM | 3541 | CG  | PRO | 487 | 21.658 | -2.329 | -1.638 | 1.00 | 0.00 | 3A4 |
| ATOM | 3542 | C   | PRO | 487 | 23.927 | -0.353 | -2.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 3543 | O   | PRO | 487 | 22.999 | 0.443  | -2.510 | 1.00 | 0.00 | 3A4 |
| ATOM | 3544 | N   | VAL | 488 | 24.915 | -0.147 | -3.541 | 1.00 | 0.00 | 3A4 |
| ATOM | 3545 | CA  | VAL | 488 | 24.946 | 1.001  | -4.417 | 1.00 | 0.00 | 3A4 |
| ATOM | 3546 | CB  | VAL | 488 | 25.614 | 2.234  | -3.794 | 1.00 | 0.00 | 3A4 |
| ATOM | 3547 | CG1 | VAL | 488 | 26.927 | 1.920  | -3.030 | 1.00 | 0.00 | 3A4 |
| ATOM | 3548 | CG2 | VAL | 488 | 25.731 | 3.431  | -4.776 | 1.00 | 0.00 | 3A4 |
| ATOM | 3549 | C   | VAL | 488 | 25.663 | 0.556  | -5.657 | 1.00 | 0.00 | 3A4 |
| ATOM | 3550 | O   | VAL | 488 | 26.886 | 0.485  | -5.692 | 1.00 | 0.00 | 3A4 |
| ATOM | 3551 | N   | VAL | 489 | 24.905 | 0.264  | -6.743 | 1.00 | 0.00 | 3A4 |
| ATOM | 3552 | CA  | VAL | 489 | 25.452 | -0.202 | -8.007 | 1.00 | 0.00 | 3A4 |
| ATOM | 3553 | CB  | VAL | 489 | 24.587 | -1.266 | -8.687 | 1.00 | 0.00 | 3A4 |
| ATOM | 3554 | CG1 | VAL | 489 | 25.369 | -1.938 | -9.848 | 1.00 | 0.00 | 3A4 |
| ATOM | 3555 | CG2 | VAL | 489 | 24.212 | -2.339 | -7.638 | 1.00 | 0.00 | 3A4 |
| ATOM | 3556 | C   | VAL | 489 | 25.702 | 0.999  | -8.916 | 1.00 | 0.00 | 3A4 |
| ATOM | 3557 | O   | VAL | 489 | 24.854 | 1.864  | -9.093 | 1.00 | 0.00 | 3A4 |

|      |      |     |     |     |        |        |         |      |      |     |
|------|------|-----|-----|-----|--------|--------|---------|------|------|-----|
| ATOM | 3558 | N   | LEU | 490 | 26.915 | 1.064  | -9.499  | 1.00 | 0.00 | 3A4 |
| ATOM | 3559 | CA  | LEU | 490 | 27.387 | 2.104  | -10.386 | 1.00 | 0.00 | 3A4 |
| ATOM | 3560 | CB  | LEU | 490 | 28.695 | 2.765  | -9.828  | 1.00 | 0.00 | 3A4 |
| ATOM | 3561 | CG  | LEU | 490 | 29.556 | 3.732  | -10.717 | 1.00 | 0.00 | 3A4 |
| ATOM | 3562 | CD1 | LEU | 490 | 30.364 | 4.675  | -9.816  | 1.00 | 0.00 | 3A4 |
| ATOM | 3563 | CD2 | LEU | 490 | 30.579 | 3.092  | -11.694 | 1.00 | 0.00 | 3A4 |
| ATOM | 3564 | C   | LEU | 490 | 27.689 | 1.443  | -11.710 | 1.00 | 0.00 | 3A4 |
| ATOM | 3565 | O   | LEU | 490 | 28.311 | 0.382  | -11.714 | 1.00 | 0.00 | 3A4 |
| ATOM | 3566 | N   | LYS | 491 | 27.223 | 2.080  | -12.824 | 1.00 | 0.00 | 3A4 |
| ATOM | 3567 | CA  | LYS | 491 | 27.177 | 1.589  | -14.188 | 1.00 | 0.00 | 3A4 |
| ATOM | 3568 | CB  | LYS | 491 | 25.982 | 2.230  | -14.965 | 1.00 | 0.00 | 3A4 |
| ATOM | 3569 | CG  | LYS | 491 | 25.687 | 1.704  | -16.388 | 1.00 | 0.00 | 3A4 |
| ATOM | 3570 | CD  | LYS | 491 | 25.319 | 0.219  | -16.460 | 1.00 | 0.00 | 3A4 |
| ATOM | 3571 | CE  | LYS | 491 | 25.043 | -0.263 | -17.889 | 1.00 | 0.00 | 3A4 |
| ATOM | 3572 | NZ  | LYS | 491 | 24.678 | -1.699 | -17.899 | 1.00 | 0.00 | 3A4 |
| ATOM | 3573 | C   | LYS | 491 | 28.494 | 1.812  | -14.912 | 1.00 | 0.00 | 3A4 |
| ATOM | 3574 | O   | LYS | 491 | 29.380 | 0.964  | -14.854 | 1.00 | 0.00 | 3A4 |
| ATOM | 3575 | N   | VAL | 492 | 28.641 | 2.966  | -15.620 | 1.00 | 0.00 | 3A4 |
| ATOM | 3576 | CA  | VAL | 492 | 29.700 | 3.255  | -16.574 | 1.00 | 0.00 | 3A4 |
| ATOM | 3577 | CB  | VAL | 492 | 29.112 | 3.889  | -17.838 | 1.00 | 0.00 | 3A4 |
| ATOM | 3578 | CG1 | VAL | 492 | 28.415 | 5.242  | -17.560 | 1.00 | 0.00 | 3A4 |
| ATOM | 3579 | CG2 | VAL | 492 | 30.130 | 3.946  | -19.001 | 1.00 | 0.00 | 3A4 |
| ATOM | 3580 | C   | VAL | 492 | 30.777 | 4.082  | -15.898 | 1.00 | 0.00 | 3A4 |
| ATOM | 3581 | O   | VAL | 492 | 30.519 | 4.769  | -14.911 | 1.00 | 0.00 | 3A4 |
| ATOM | 3582 | N   | GLU | 493 | 32.030 | 3.983  | -16.415 | 1.00 | 0.00 | 3A4 |
| ATOM | 3583 | CA  | GLU | 493 | 33.215 | 4.574  | -15.836 | 1.00 | 0.00 | 3A4 |
| ATOM | 3584 | CB  | GLU | 493 | 33.962 | 3.566  | -14.901 | 1.00 | 0.00 | 3A4 |
| ATOM | 3585 | CG  | GLU | 493 | 34.397 | 2.206  | -15.502 | 1.00 | 0.00 | 3A4 |
| ATOM | 3586 | CD  | GLU | 493 | 35.792 | 2.272  | -16.141 | 1.00 | 0.00 | 3A4 |
| ATOM | 3587 | OE1 | GLU | 493 | 36.769 | 2.568  | -15.402 | 1.00 | 0.00 | 3A4 |
| ATOM | 3588 | OE2 | GLU | 493 | 35.901 | 2.024  | -17.372 | 1.00 | 0.00 | 3A4 |
| ATOM | 3589 | C   | GLU | 493 | 34.100 | 5.031  | -16.967 | 1.00 | 0.00 | 3A4 |
| ATOM | 3590 | O   | GLU | 493 | 33.928 | 4.629  | -18.117 | 1.00 | 0.00 | 3A4 |
| ATOM | 3591 | N   | SER | 494 | 35.109 | 5.874  | -16.624 | 1.00 | 0.00 | 3A4 |
| ATOM | 3592 | CA  | SER | 494 | 36.209 | 6.283  | -17.480 | 1.00 | 0.00 | 3A4 |
| ATOM | 3593 | CB  | SER | 494 | 36.076 | 7.748  | -18.010 | 1.00 | 0.00 | 3A4 |
| ATOM | 3594 | OG  | SER | 494 | 35.765 | 8.692  | -16.990 | 1.00 | 0.00 | 3A4 |
| ATOM | 3595 | C   | SER | 494 | 37.455 | 6.059  | -16.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 3596 | O   | SER | 494 | 37.360 | 5.784  | -15.452 | 1.00 | 0.00 | 3A4 |
| ATOM | 3597 | N   | ARG | 495 | 38.664 | 6.138  | -17.262 | 1.00 | 0.00 | 3A4 |
| ATOM | 3598 | CA  | ARG | 495 | 39.886 | 5.740  | -16.587 | 1.00 | 0.00 | 3A4 |
| ATOM | 3599 | CB  | ARG | 495 | 40.090 | 4.192  | -16.590 | 1.00 | 0.00 | 3A4 |
| ATOM | 3600 | CG  | ARG | 495 | 39.845 | 3.452  | -17.916 | 1.00 | 0.00 | 3A4 |
| ATOM | 3601 | CD  | ARG | 495 | 39.764 | 1.935  | -17.697 | 1.00 | 0.00 | 3A4 |
| ATOM | 3602 | NE  | ARG | 495 | 39.301 | 1.272  | -18.966 | 1.00 | 0.00 | 3A4 |
| ATOM | 3603 | CZ  | ARG | 495 | 38.710 | 0.032  | -18.992 | 1.00 | 0.00 | 3A4 |
| ATOM | 3604 | NH1 | ARG | 495 | 38.289 | -0.478 | -20.185 | 1.00 | 0.00 | 3A4 |
| ATOM | 3605 | NH2 | ARG | 495 | 38.527 | -0.702 | -17.853 | 1.00 | 0.00 | 3A4 |
| ATOM | 3606 | C   | ARG | 495 | 41.073 | 6.436  | -17.202 | 1.00 | 0.00 | 3A4 |
| ATOM | 3607 | O   | ARG | 495 | 41.144 | 6.643  | -18.413 | 1.00 | 0.00 | 3A4 |
| ATOM | 3608 | N   | ASP | 496 | 42.044 | 6.804  | -16.320 | 1.00 | 0.00 | 3A4 |
| ATOM | 3609 | CA  | ASP | 496 | 43.290 | 7.471  | -16.647 | 1.00 | 0.00 | 3A4 |
| ATOM | 3610 | CB  | ASP | 496 | 43.159 | 9.025  | -16.860 | 1.00 | 0.00 | 3A4 |
| ATOM | 3611 | CG  | ASP | 496 | 42.410 | 9.788  | -15.743 | 1.00 | 0.00 | 3A4 |
| ATOM | 3612 | OD1 | ASP | 496 | 43.070 | 10.614 | -15.056 | 1.00 | 0.00 | 3A4 |
| ATOM | 3613 | OD2 | ASP | 496 | 41.179 | 9.574  | -15.577 | 1.00 | 0.00 | 3A4 |
| ATOM | 3614 | C   | ASP | 496 | 44.272 | 7.071  | -15.553 | 1.00 | 0.00 | 3A4 |
| ATOM | 3615 | O   | ASP | 496 | 44.432 | 5.882  | -15.283 | 1.00 | 0.00 | 3A4 |
| ATOM | 3616 | N   | GLY | 497 | 44.958 | 8.050  | -14.898 | 1.00 | 0.00 | 3A4 |
| ATOM | 3617 | CA  | GLY | 497 | 45.950 | 7.790  | -13.872 | 1.00 | 0.00 | 3A4 |
| ATOM | 3618 | C   | GLY | 497 | 46.123 | 9.024  | -13.031 | 1.00 | 0.00 | 3A4 |
| ATOM | 3619 | O   | GLY | 497 | 46.262 | 10.127 | -13.557 | 1.00 | 0.00 | 3A4 |
| ATOM | 3620 | N   | THR | 498 | 46.127 | 8.846  | -11.677 | 1.00 | 0.00 | 3A4 |
| ATOM | 3621 | CA  | THR | 498 | 46.355 | 9.879  | -10.674 | 1.00 | 0.00 | 3A4 |
| ATOM | 3622 | CB  | THR | 498 | 45.075 | 10.401 | -9.995  | 1.00 | 0.00 | 3A4 |
| ATOM | 3623 | OG1 | THR | 498 | 44.194 | 9.349  | -9.600  | 1.00 | 0.00 | 3A4 |
| ATOM | 3624 | CG2 | THR | 498 | 44.332 | 11.355 | -10.957 | 1.00 | 0.00 | 3A4 |
| ATOM | 3625 | C   | THR | 498 | 47.290 | 9.274  | -9.640  | 1.00 | 0.00 | 3A4 |
| ATOM | 3626 | O   | THR | 498 | 47.189 | 8.089  | -9.326  | 1.00 | 0.00 | 3A4 |
| ATOM | 3627 | N   | VAL | 499 | 48.205 | 10.109 | -9.074  | 1.00 | 0.00 | 3A4 |
| ATOM | 3628 | CA  | VAL | 499 | 49.121 | 9.727  | -8.014  | 1.00 | 0.00 | 3A4 |
| ATOM | 3629 | CB  | VAL | 499 | 50.272 | 8.816  | -8.476  | 1.00 | 0.00 | 3A4 |

|        |      |     |     |     |        |        |        |      |      |     |
|--------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM   | 3630 | CG1 | VAL | 499 | 51.133 | 9.436  | -9.607 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3631 | CG2 | VAL | 499 | 51.110 | 8.313  | -7.273 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3632 | C   | VAL | 499 | 49.614 | 11.021 | -7.391 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3633 | O   | VAL | 499 | 49.977 | 11.961 | -8.097 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3634 | N   | SER | 500 | 49.647 | 11.075 | -6.030 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3635 | CA  | SER | 500 | 50.251 | 12.152 | -5.269 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3636 | CB  | SER | 500 | 49.434 | 13.486 | -5.230 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3637 | OG  | SER | 500 | 48.086 | 13.306 | -4.816 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3638 | C   | SER | 500 | 50.524 | 11.618 | -3.882 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3639 | O   | SER | 500 | 49.694 | 10.933 | -3.286 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3640 | N   | GLY | 501 | 51.736 | 11.945 | -3.355 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3641 | CA  | GLY | 501 | 52.249 | 11.543 | -2.061 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3642 | C   | GLY | 501 | 53.489 | 10.727 | -2.291 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3643 | O   | GLY | 501 | 54.576 | 11.087 | -1.841 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3644 | N   | ALA | 502 | 53.331 | 9.596  | -3.020 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3645 | CA  | ALA | 502 | 54.406 | 8.722  | -3.424 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3646 | CB  | ALA | 502 | 54.772 | 7.642  | -2.379 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3647 | C   | ALA | 502 | 53.912 | 8.031  | -4.704 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3648 | OT1 | ALA | 502 | 54.439 | 8.364  | -5.800 | 1.00 | 0.00 | 3A4 |
| ATOM   | 3649 | OT2 | ALA | 502 | 52.987 | 7.178  | -4.607 | 1.00 | 0.00 | 3A4 |
| TER    | 3650 |     | ALA | 502 |        |        |        |      |      |     |
| HETATM | 3651 | FE  | HEM | 600 | 33.118 | 10.391 | 15.288 | 1.00 | 0.00 | HEM |
| HETATM | 3652 | NA  | HEM | 600 | 31.497 | 11.115 | 16.171 | 1.00 | 0.00 | HEM |
| HETATM | 3653 | NB  | HEM | 600 | 32.274 | 10.658 | 13.514 | 1.00 | 0.00 | HEM |
| HETATM | 3654 | NC  | HEM | 600 | 34.752 | 9.684  | 14.430 | 1.00 | 0.00 | HEM |
| HETATM | 3655 | ND  | HEM | 600 | 33.949 | 10.106 | 17.065 | 1.00 | 0.00 | HEM |
| HETATM | 3656 | C1A | HEM | 600 | 31.254 | 11.251 | 17.515 | 1.00 | 0.00 | HEM |
| HETATM | 3657 | C2A | HEM | 600 | 29.887 | 11.659 | 17.752 | 1.00 | 0.00 | HEM |
| HETATM | 3658 | C3A | HEM | 600 | 29.316 | 11.871 | 16.542 | 1.00 | 0.00 | HEM |
| HETATM | 3659 | C4A | HEM | 600 | 30.322 | 11.523 | 15.568 | 1.00 | 0.00 | HEM |
| HETATM | 3660 | C1B | HEM | 600 | 31.012 | 11.136 | 13.233 | 1.00 | 0.00 | HEM |
| HETATM | 3661 | C2B | HEM | 600 | 30.761 | 11.218 | 11.804 | 1.00 | 0.00 | HEM |
| HETATM | 3662 | C3B | HEM | 600 | 31.901 | 10.761 | 11.185 | 1.00 | 0.00 | HEM |
| HETATM | 3663 | C4B | HEM | 600 | 32.828 | 10.426 | 12.273 | 1.00 | 0.00 | HEM |
| HETATM | 3664 | C1C | HEM | 600 | 35.044 | 9.645  | 13.089 | 1.00 | 0.00 | HEM |
| HETATM | 3665 | C2C | HEM | 600 | 36.395 | 9.168  | 12.838 | 1.00 | 0.00 | HEM |
| HETATM | 3666 | C3C | HEM | 600 | 36.920 | 8.833  | 14.067 | 1.00 | 0.00 | HEM |
| HETATM | 3667 | C4C | HEM | 600 | 35.879 | 9.167  | 15.033 | 1.00 | 0.00 | HEM |
| HETATM | 3668 | C1D | HEM | 600 | 35.150 | 9.494  | 17.358 | 1.00 | 0.00 | HEM |
| HETATM | 3669 | C2D | HEM | 600 | 35.382 | 9.408  | 18.787 | 1.00 | 0.00 | HEM |
| HETATM | 3670 | C3D | HEM | 600 | 34.329 | 10.035 | 19.375 | 1.00 | 0.00 | HEM |
| HETATM | 3671 | C4D | HEM | 600 | 33.438 | 10.439 | 18.306 | 1.00 | 0.00 | HE  |

**Table 4:** Providing the coordinates of the CYP3A model

| HEADER | CYP3A7   |
|--------|--|
| TITLE  | MODEL OF HUMAN CYTOCHROME P450 CYP3A7                                |
| AUTHOR | N. LOISEAU, F. ANDRE, M. DELAFORGE, M. COTTEVIEILLE                  |
| SEQRES | 1 459 PRO PHE LEU GLY ASN ALA LEU SER PHE ARG LYS GLY TYR            |
| SEQRES | 2 459 TRP THR PHE ASP MET GLU CYS TYR LYS LYS TYR ARG LYS            |
| SEQRES | 3 459 VAL TRP GLY ILE TYR ASP CYS GLN GLN PRO MET LEU ALA            |
| SEQRES | 4 459 ILE THR ASP PRO ASP MET ILE LYS THR VAL LEU VAL LYS            |
| SEQRES | 5 459 GLU CYS TYR SER VAL PHE THR ASN ARG ARG PRO PHE GLY            |
| SEQRES | 6 459 PRO VAL GLY PHE MET LYS ASN ALA ILE SER ILE ALA GLU            |
| SEQRES | 7 459 ASP GLU GLU TRP LYS ARG ILE ARG SER LEU LEU SER PRO            |
| SEQRES | 8 459 THR PHE THR SER GLY LYS LEU LYS GLU MET VAL PRO ILE            |
| SEQRES | 9 459 ILE ALA GLN TYR GLY ASP VAL LEU VAL ARG ASN LEU ARG            |
| SEQRES | 10 459 ARG GLU ALA GLU THR GLY LYS PRO VAL THR LEU LYS HIS           |
| SEQRES | 11 459 VAL PHE GLY ALA TYR SER MET ASP VAL ILE THR SER THR           |
| SEQRES | 12 459 SER PHE GLY VAL SER ILE ASP SER LEU ASN ASN PRO GLN           |
| SEQRES | 13 459 ASP PRO PHE VAL GLU ASN THR LYS LYS LEU LEU ARG PHE           |
| SEQRES | 14 459 ASN PRO LEU ASP PRO PHE VAL LEU SER ILE LYS VAL PHE           |
| SEQRES | 15 459 PRO PHE LEU THR PRO ILE LEU GLU ALA LEU ASN ILE THR           |
| SEQRES | 16 459 VAL PHE PRO ARG LYS VAL ILE SER PHE LEU THR LYS SER           |
| SEQRES | 17 459 VAL LYS GLN ILE LYS GLU GLY ARG LEU LYS GLU THR GLN           |
| SEQRES | 18 459 LYS HIS ARG VAL ASP PHE LEU GLN LEU MET ILE ASP SER           |
| SEQRES | 19 459 GLN ASN SER LYS ASP SER GLU THR HIS LYS ALA LEU SER           |
| SEQRES | 20 459 ASP LEU GLU LEU MET ALA GLN SER ILE ILE PHE ILE PHE           |
| SEQRES | 21 459 ALA GLY TYR GLU THR THR SER SER VAL LEU SER PHE ILE           |
| SEQRES | 22 459 ILE TYR GLU LEU ALA THR HIS PRO ASP VAL GLN GLN LYS           |
| SEQRES | 23 459 VAL GLN LYS GLU ILE ASP THR VAL LEU PRO ASN LYS ALA           |
| SEQRES | 24 459 PRO PRO THR TYR ASP THR VAL LEU GLN LEU GLU TYR LEU           |
| SEQRES | 25 459 ASP MET VAL VAL ASN GLU THR LEU ARG LEU PHE PRO VAL           |
| SEQRES | 26 459 ALA MET ARG LEU GLU ARG VAL CYS LYS LYS ASP VAL GLU           |
| SEQRES | 27 459 ILE ASN GLY MET PHE ILE PRO LYS GLY VAL VAL VAL MET           |
| SEQRES | 28 459 ILE PRO SER TYR VAL LEU HIS HIS ASP PRO LYS TYR TRP           |
| SEQRES | 29 459 THR GLU PRO GLU LYS PHE LEU PRO GLU ARG PHE SER LYS           |
| SEQRES | 30 459 LYS ASN LYS ASP ASN ILE ASP PRO TYR ILE TYR THR PRO           |
| SEQRES | 31 459 PHE GLY SER GLY PRO ARG ASN CYS ILE GLY MET ARG PHE           |
| SEQRES | 32 459 ALA LEU VAL ASN MET LYS LEU ALA LEU VAL ARG VAL LEU           |
| SEQRES | 33 459 GLN ASN PHE SER PHE LYS PRO CYS LYS GLU THR GLN ILE           |
| SEQRES | 34 459 PRO LEU LYS LEU ARG PHE GLY GLY LEU LEU LEU THR GLU           |
| SEQRES | 35 459 LYS PRO ILE VAL LEU LYS ALA GLU SER ARG ASP GLU THR           |
| SEQRES | 36 459 VAL SER GLY ALA   |
| HET    | HEM 600  |
| HETNAM | HEM HEME   |
| HETSYN | HEM 3,7,12,17-TETRAMETHYL-8,13-DIVINYL-2,18-PORPHINEDIPROPIONIC ACID |
| FORMUL | HEM C34 H34 N4 O4 FE1  |
| ATOM   | 1 N PRO 45 24.768 6.244 -5.895 1.00 0.00 3A7                         |
| ATOM   | 2 CD PRO 45 25.053 5.448 -4.648 1.00 0.00 3A7                        |
| ATOM   | 3 CA PRO 45 24.705 5.319 -7.064 1.00 0.00 3A7                        |
| ATOM   | 4 CB PRO 45 24.467 3.950 -6.422 1.00 0.00 3A7                        |
| ATOM   | 5 CG PRO 45 25.292 4.018 -5.139 1.00 0.00 3A7                        |
| ATOM   | 6 C PRO 45 23.594 5.801 -7.950 1.00 0.00 3A7                         |
| ATOM   | 7 O PRO 45 23.387 7.010 -8.057 1.00 0.00 3A7                         |
| ATOM   | 8 N PHE 46 22.870 4.857 -8.600 1.00 0.00 3A7                         |
| ATOM   | 9 CA PHE 46 21.751 5.140 -9.472 1.00 0.00 3A7                        |
| ATOM   | 10 CB PHE 46 21.853 4.416 -10.835 1.00 0.00 3A7                      |
| ATOM   | 11 CG PHE 46 23.083 4.887 -11.553 1.00 0.00 3A7                      |
| ATOM   | 12 CD1 PHE 46 24.173 4.033 -11.730 1.00 0.00 3A7                     |
| ATOM   | 13 CD2 PHE 46 23.155 6.189 -12.049 1.00 0.00 3A7                     |
| ATOM   | 14 CE1 PHE 46 25.317 4.474 -12.390 1.00 0.00 3A7                     |
| ATOM   | 15 CE2 PHE 46 24.297 6.633 -12.709 1.00 0.00 3A7                     |
| ATOM   | 16 CZ PHE 46 25.380 5.775 -12.879 1.00 0.00 3A7                      |
| ATOM   | 17 C PHE 46 20.491 4.691 -8.782 1.00 0.00 3A7                        |
| ATOM   | 18 O PHE 46 19.400 5.166 -9.096 1.00 0.00 3A7                        |
| ATOM   | 19 N LEU 47 20.629 3.749 -7.814 1.00 0.00 3A7                        |
| ATOM   | 20 CA LEU 47 19.541 3.204 -7.035 1.00 0.00 3A7                       |
| ATOM   | 21 CB LEU 47 19.661 1.667 -6.874 1.00 0.00 3A7                       |
| ATOM   | 22 CG LEU 47 18.490 0.978 -6.129 1.00 0.00 3A7                       |
| ATOM   | 23 CD1 LEU 47 17.133 1.202 -6.826 1.00 0.00 3A7                      |
| ATOM   | 24 CD2 LEU 47 18.768 -0.526 -5.942 1.00 0.00 3A7                     |
| ATOM   | 25 C LEU 47 19.573 3.860 -5.681 1.00 0.00 3A7                        |
| ATOM   | 26 O LEU 47 20.619 3.930 -5.036 1.00 0.00 3A7                        |
| ATOM   | 27 N GLY 48 18.396 4.349 -5.225 1.00 0.00 3A7                        |
| ATOM   | 28 CA GLY 48 18.240 4.966 -3.933 1.00 0.00 3A7                       |

|      |     |     |     |    |        |         |        |      |      |     |
|------|-----|-----|-----|----|--------|---------|--------|------|------|-----|
| ATOM | 29  | C   | GLY | 48 | 16.930 | 4.491   | -3.395 | 1.00 | 0.00 | 3A7 |
| ATOM | 30  | O   | GLY | 48 | 15.938 | 5.218   | -3.414 | 1.00 | 0.00 | 3A7 |
| ATOM | 31  | N   | ASN | 49 | 16.911 | 3.229   | -2.898 | 1.00 | 0.00 | 3A7 |
| ATOM | 32  | CA  | ASN | 49 | 15.741 | 2.585   | -2.348 | 1.00 | 0.00 | 3A7 |
| ATOM | 33  | CB  | ASN | 49 | 15.445 | 1.235   | -3.059 | 1.00 | 0.00 | 3A7 |
| ATOM | 34  | CG  | ASN | 49 | 14.046 | 0.705   | -2.706 | 1.00 | 0.00 | 3A7 |
| ATOM | 35  | OD1 | ASN | 49 | 13.035 | 1.349   | -3.011 | 1.00 | 0.00 | 3A7 |
| ATOM | 36  | ND2 | ASN | 49 | 14.005 | -0.494  | -2.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 37  | C   | ASN | 49 | 16.016 | 2.375   | -0.880 | 1.00 | 0.00 | 3A7 |
| ATOM | 38  | O   | ASN | 49 | 17.169 | 2.278   | -0.463 | 1.00 | 0.00 | 3A7 |
| ATOM | 39  | N   | ALA | 50 | 14.933 | 2.293   | -0.065 | 1.00 | 0.00 | 3A7 |
| ATOM | 40  | CA  | ALA | 50 | 14.998 | 2.111   | 1.369  | 1.00 | 0.00 | 3A7 |
| ATOM | 41  | CB  | ALA | 50 | 13.847 | 2.834   | 2.098  | 1.00 | 0.00 | 3A7 |
| ATOM | 42  | C   | ALA | 50 | 14.941 | 0.641   | 1.697  | 1.00 | 0.00 | 3A7 |
| ATOM | 43  | O   | ALA | 50 | 13.866 | 0.049   | 1.787  | 1.00 | 0.00 | 3A7 |
| ATOM | 44  | N   | LEU | 51 | 16.133 | 0.032   | 1.885  | 1.00 | 0.00 | 3A7 |
| ATOM | 45  | CA  | LEU | 51 | 16.271 | -1.360  | 2.232  | 1.00 | 0.00 | 3A7 |
| ATOM | 46  | CB  | LEU | 51 | 16.271 | -2.314  | 1.001  | 1.00 | 0.00 | 3A7 |
| ATOM | 47  | CG  | LEU | 51 | 17.055 | -1.862  | -0.262 | 1.00 | 0.00 | 3A7 |
| ATOM | 48  | CD1 | LEU | 51 | 18.587 | -1.811  | -0.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 49  | CD2 | LEU | 51 | 16.690 | -2.765  | -1.456 | 1.00 | 0.00 | 3A7 |
| ATOM | 50  | C   | LEU | 51 | 17.550 | -1.468  | 3.012  | 1.00 | 0.00 | 3A7 |
| ATOM | 51  | O   | LEU | 51 | 18.327 | -0.517  | 3.085  | 1.00 | 0.00 | 3A7 |
| ATOM | 52  | N   | SER | 52 | 17.794 | -2.657  | 3.613  | 1.00 | 0.00 | 3A7 |
| ATOM | 53  | CA  | SER | 52 | 19.005 | -2.956  | 4.343  | 1.00 | 0.00 | 3A7 |
| ATOM | 54  | CB  | SER | 52 | 18.741 | -3.361  | 5.821  | 1.00 | 0.00 | 3A7 |
| ATOM | 55  | OG  | SER | 52 | 17.737 | -4.363  | 5.945  | 1.00 | 0.00 | 3A7 |
| ATOM | 56  | C   | SER | 52 | 19.734 | -4.023  | 3.562  | 1.00 | 0.00 | 3A7 |
| ATOM | 57  | O   | SER | 52 | 20.164 | -3.782  | 2.435  | 1.00 | 0.00 | 3A7 |
| ATOM | 58  | N   | PHE | 53 | 19.898 | -5.231  | 4.155  | 1.00 | 0.00 | 3A7 |
| ATOM | 59  | CA  | PHE | 53 | 20.599 | -6.341  | 3.550  | 1.00 | 0.00 | 3A7 |
| ATOM | 60  | CB  | PHE | 53 | 21.908 | -6.703  | 4.297  | 1.00 | 0.00 | 3A7 |
| ATOM | 61  | CG  | PHE | 53 | 22.730 | -5.456  | 4.439  | 1.00 | 0.00 | 3A7 |
| ATOM | 62  | CD1 | PHE | 53 | 22.819 | -4.809  | 5.673  | 1.00 | 0.00 | 3A7 |
| ATOM | 63  | CD2 | PHE | 53 | 23.346 | -4.880  | 3.327  | 1.00 | 0.00 | 3A7 |
| ATOM | 64  | CE1 | PHE | 53 | 23.491 | -3.598  | 5.793  | 1.00 | 0.00 | 3A7 |
| ATOM | 65  | CE2 | PHE | 53 | 24.018 | -3.667  | 3.446  | 1.00 | 0.00 | 3A7 |
| ATOM | 66  | CZ  | PHE | 53 | 24.085 | -3.022  | 4.675  | 1.00 | 0.00 | 3A7 |
| ATOM | 67  | C   | PHE | 53 | 19.639 | -7.494  | 3.594  | 1.00 | 0.00 | 3A7 |
| ATOM | 68  | O   | PHE | 53 | 19.885 | -8.495  | 4.264  | 1.00 | 0.00 | 3A7 |
| ATOM | 69  | N   | ARG | 54 | 18.491 | -7.330  | 2.875  | 1.00 | 0.00 | 3A7 |
| ATOM | 70  | CA  | ARG | 54 | 17.327 | -8.205  | 2.828  | 1.00 | 0.00 | 3A7 |
| ATOM | 71  | CB  | ARG | 54 | 17.629 | -9.719  | 2.641  | 1.00 | 0.00 | 3A7 |
| ATOM | 72  | CG  | ARG | 54 | 18.536 | -10.045 | 1.437  | 1.00 | 0.00 | 3A7 |
| ATOM | 73  | CD  | ARG | 54 | 17.996 | -9.573  | 0.079  | 1.00 | 0.00 | 3A7 |
| ATOM | 74  | NE  | ARG | 54 | 19.049 | -9.836  | -0.962 | 1.00 | 0.00 | 3A7 |
| ATOM | 75  | CZ  | ARG | 54 | 19.036 | -10.925 | -1.791 | 1.00 | 0.00 | 3A7 |
| ATOM | 76  | NH1 | ARG | 54 | 20.065 | -11.113 | -2.669 | 1.00 | 0.00 | 3A7 |
| ATOM | 77  | NH2 | ARG | 54 | 18.013 | -11.826 | -1.753 | 1.00 | 0.00 | 3A7 |
| ATOM | 78  | C   | ARG | 54 | 16.514 | -7.983  | 4.087  | 1.00 | 0.00 | 3A7 |
| ATOM | 79  | O   | ARG | 54 | 16.760 | -8.611  | 5.116  | 1.00 | 0.00 | 3A7 |
| ATOM | 80  | N   | LYS | 55 | 15.545 | -7.030  | 4.028  | 1.00 | 0.00 | 3A7 |
| ATOM | 81  | CA  | LYS | 55 | 14.927 | -6.447  | 5.205  | 1.00 | 0.00 | 3A7 |
| ATOM | 82  | CB  | LYS | 55 | 14.520 | -4.971  | 5.023  | 1.00 | 0.00 | 3A7 |
| ATOM | 83  | CG  | LYS | 55 | 13.327 | -4.656  | 4.092  | 1.00 | 0.00 | 3A7 |
| ATOM | 84  | CD  | LYS | 55 | 13.574 | -4.842  | 2.582  | 1.00 | 0.00 | 3A7 |
| ATOM | 85  | CE  | LYS | 55 | 13.074 | -6.171  | 1.993  | 1.00 | 0.00 | 3A7 |
| ATOM | 86  | NZ  | LYS | 55 | 11.612 | -6.322  | 2.178  | 1.00 | 0.00 | 3A7 |
| ATOM | 87  | C   | LYS | 55 | 13.767 | -7.241  | 5.777  | 1.00 | 0.00 | 3A7 |
| ATOM | 88  | O   | LYS | 55 | 13.403 | -7.067  | 6.938  | 1.00 | 0.00 | 3A7 |
| ATOM | 89  | N   | GLY | 56 | 13.158 | -8.146  | 4.991  | 1.00 | 0.00 | 3A7 |
| ATOM | 90  | CA  | GLY | 56 | 12.066 | -8.950  | 5.491  | 1.00 | 0.00 | 3A7 |
| ATOM | 91  | C   | GLY | 56 | 11.995 | -10.146 | 4.604  | 1.00 | 0.00 | 3A7 |
| ATOM | 92  | O   | GLY | 56 | 11.061 | -10.334 | 3.823  | 1.00 | 0.00 | 3A7 |
| ATOM | 93  | N   | TYR | 57 | 13.009 | -11.031 | 4.730  | 1.00 | 0.00 | 3A7 |
| ATOM | 94  | CA  | TYR | 57 | 13.171 | -12.222 | 3.922  | 1.00 | 0.00 | 3A7 |
| ATOM | 95  | CB  | TYR | 57 | 14.496 | -12.913 | 4.319  | 1.00 | 0.00 | 3A7 |
| ATOM | 96  | CG  | TYR | 57 | 15.183 | -13.558 | 3.146  | 1.00 | 0.00 | 3A7 |
| ATOM | 97  | CD1 | TYR | 57 | 15.496 | -12.832 | 1.995  | 1.00 | 0.00 | 3A7 |
| ATOM | 98  | CD2 | TYR | 57 | 15.566 | -14.898 | 3.223  | 1.00 | 0.00 | 3A7 |
| ATOM | 99  | CE1 | TYR | 57 | 16.160 | -13.440 | 0.934  | 1.00 | 0.00 | 3A7 |
| ATOM | 100 | CE2 | TYR | 57 | 16.240 | -15.506 | 2.168  | 1.00 | 0.00 | 3A7 |

|      |     |     |     |    |        |         |        |      |      |     |
|------|-----|-----|-----|----|--------|---------|--------|------|------|-----|
| ATOM | 101 | CZ  | TYR | 57 | 16.538 | -14.777 | 1.021  | 1.00 | 0.00 | 3A7 |
| ATOM | 102 | OH  | TYR | 57 | 17.229 | -15.392 | -0.043 | 1.00 | 0.00 | 3A7 |
| ATOM | 103 | C   | TYR | 57 | 12.013 | -13.191 | 4.022  | 1.00 | 0.00 | 3A7 |
| ATOM | 104 | O   | TYR | 57 | 11.631 | -13.781 | 3.021  | 1.00 | 0.00 | 3A7 |
| ATOM | 105 | N   | TRP | 58 | 11.379 | -13.353 | 5.211  | 1.00 | 0.00 | 3A7 |
| ATOM | 106 | CA  | TRP | 58 | 10.261 | -14.269 | 5.359  | 1.00 | 0.00 | 3A7 |
| ATOM | 107 | CB  | TRP | 58 | 9.872  | -14.515 | 6.832  | 1.00 | 0.00 | 3A7 |
| ATOM | 108 | CG  | TRP | 58 | 9.333  | -13.318 | 7.606  | 1.00 | 0.00 | 3A7 |
| ATOM | 109 | CD2 | TRP | 58 | 8.006  | -13.247 | 8.157  | 1.00 | 0.00 | 3A7 |
| ATOM | 110 | CD1 | TRP | 58 | 9.925  | -12.115 | 7.871  | 1.00 | 0.00 | 3A7 |
| ATOM | 111 | NE1 | TRP | 58 | 9.051  | -11.297 | 8.548  | 1.00 | 0.00 | 3A7 |
| ATOM | 112 | CE2 | TRP | 58 | 7.869  | -11.978 | 8.741  | 1.00 | 0.00 | 3A7 |
| ATOM | 113 | CE3 | TRP | 58 | 6.969  | -14.158 | 8.175  | 1.00 | 0.00 | 3A7 |
| ATOM | 114 | CZ2 | TRP | 58 | 6.694  | -11.604 | 9.360  | 1.00 | 0.00 | 3A7 |
| ATOM | 115 | CZ3 | TRP | 58 | 5.782  | -13.780 | 8.796  | 1.00 | 0.00 | 3A7 |
| ATOM | 116 | CH2 | TRP | 58 | 5.647  | -12.522 | 9.382  | 1.00 | 0.00 | 3A7 |
| ATOM | 117 | C   | TRP | 58 | 9.036  | -13.824 | 4.612  | 1.00 | 0.00 | 3A7 |
| ATOM | 118 | O   | TRP | 58 | 8.302  | -14.664 | 4.106  | 1.00 | 0.00 | 3A7 |
| ATOM | 119 | N   | THR | 59 | 8.780  | -12.490 | 4.502  | 1.00 | 0.00 | 3A7 |
| ATOM | 120 | CA  | THR | 59 | 7.645  | -11.989 | 3.737  | 1.00 | 0.00 | 3A7 |
| ATOM | 121 | CB  | THR | 59 | 7.213  | -10.582 | 4.136  | 1.00 | 0.00 | 3A7 |
| ATOM | 122 | OG1 | THR | 59 | 8.282  | -9.643  | 4.073  | 1.00 | 0.00 | 3A7 |
| ATOM | 123 | CG2 | THR | 59 | 6.673  | -10.634 | 5.579  | 1.00 | 0.00 | 3A7 |
| ATOM | 124 | C   | THR | 59 | 7.925  | -12.067 | 2.267  | 1.00 | 0.00 | 3A7 |
| ATOM | 125 | O   | THR | 59 | 7.011  | -12.232 | 1.471  | 1.00 | 0.00 | 3A7 |
| ATOM | 126 | N   | PHE | 60 | 9.218  | -12.018 | 1.884  | 1.00 | 0.00 | 3A7 |
| ATOM | 127 | CA  | PHE | 60 | 9.659  | -12.244 | 0.530  | 1.00 | 0.00 | 3A7 |
| ATOM | 128 | CB  | PHE | 60 | 11.132 | -11.803 | 0.330  | 1.00 | 0.00 | 3A7 |
| ATOM | 129 | CG  | PHE | 60 | 11.512 | -11.735 | -1.126 | 1.00 | 0.00 | 3A7 |
| ATOM | 130 | CD1 | PHE | 60 | 10.889 | -10.822 | -1.978 | 1.00 | 0.00 | 3A7 |
| ATOM | 131 | CD2 | PHE | 60 | 12.481 | -12.595 | -1.647 | 1.00 | 0.00 | 3A7 |
| ATOM | 132 | CE1 | PHE | 60 | 11.222 | -10.772 | -3.328 | 1.00 | 0.00 | 3A7 |
| ATOM | 133 | CE2 | PHE | 60 | 12.816 | -12.548 | -2.997 | 1.00 | 0.00 | 3A7 |
| ATOM | 134 | CZ  | PHE | 60 | 12.186 | -11.636 | -3.839 | 1.00 | 0.00 | 3A7 |
| ATOM | 135 | C   | PHE | 60 | 9.505  | -13.695 | 0.122  | 1.00 | 0.00 | 3A7 |
| ATOM | 136 | O   | PHE | 60 | 8.967  | -14.011 | -0.936 | 1.00 | 0.00 | 3A7 |
| ATOM | 137 | N   | ASP | 61 | 9.940  | -14.632 | 0.991  | 1.00 | 0.00 | 3A7 |
| ATOM | 138 | CA  | ASP | 61 | 9.855  | -16.051 | 0.737  | 1.00 | 0.00 | 3A7 |
| ATOM | 139 | CB  | ASP | 61 | 10.621 | -16.892 | 1.774  | 1.00 | 0.00 | 3A7 |
| ATOM | 140 | CG  | ASP | 61 | 12.134 | -16.729 | 1.612  | 1.00 | 0.00 | 3A7 |
| ATOM | 141 | OD1 | ASP | 61 | 12.612 | -16.736 | 0.447  | 1.00 | 0.00 | 3A7 |
| ATOM | 142 | OD2 | ASP | 61 | 12.818 | -16.555 | 2.655  | 1.00 | 0.00 | 3A7 |
| ATOM | 143 | C   | ASP | 61 | 8.415  | -16.503 | 0.698  | 1.00 | 0.00 | 3A7 |
| ATOM | 144 | O   | ASP | 61 | 8.070  | -17.371 | -0.085 | 1.00 | 0.00 | 3A7 |
| ATOM | 145 | N   | MET | 62 | 7.521  | -15.870 | 1.491  | 1.00 | 0.00 | 3A7 |
| ATOM | 146 | CA  | MET | 62 | 6.098  | -16.134 | 1.452  | 1.00 | 0.00 | 3A7 |
| ATOM | 147 | CB  | MET | 62 | 5.374  | -15.468 | 2.623  | 1.00 | 0.00 | 3A7 |
| ATOM | 148 | CG  | MET | 62 | 5.596  | -16.224 | 3.947  | 1.00 | 0.00 | 3A7 |
| ATOM | 149 | SD  | MET | 62 | 4.969  | -15.359 | 5.422  | 1.00 | 0.00 | 3A7 |
| ATOM | 150 | CE  | MET | 62 | 3.199  | -15.481 | 5.031  | 1.00 | 0.00 | 3A7 |
| ATOM | 151 | C   | MET | 62 | 5.450  | -15.672 | 0.168  | 1.00 | 0.00 | 3A7 |
| ATOM | 152 | O   | MET | 62 | 4.555  | -16.335 | -0.342 | 1.00 | 0.00 | 3A7 |
| ATOM | 153 | N   | GLU | 63 | 5.922  | -14.555 | -0.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 154 | CA  | GLU | 63 | 5.457  | -14.094 | -1.722 | 1.00 | 0.00 | 3A7 |
| ATOM | 155 | CB  | GLU | 63 | 5.987  | -12.683 | -2.039 | 1.00 | 0.00 | 3A7 |
| ATOM | 156 | CG  | GLU | 63 | 5.290  | -11.593 | -1.206 | 1.00 | 0.00 | 3A7 |
| ATOM | 157 | CD  | GLU | 63 | 5.961  | -10.239 | -1.427 | 1.00 | 0.00 | 3A7 |
| ATOM | 158 | OE1 | GLU | 63 | 6.943  | -10.169 | -2.214 | 1.00 | 0.00 | 3A7 |
| ATOM | 159 | OE2 | GLU | 63 | 5.495  | -9.249  | -0.802 | 1.00 | 0.00 | 3A7 |
| ATOM | 160 | C   | GLU | 63 | 5.865  | -15.044 | -2.831 | 1.00 | 0.00 | 3A7 |
| ATOM | 161 | O   | GLU | 63 | 5.087  | -15.339 | -3.734 | 1.00 | 0.00 | 3A7 |
| ATOM | 162 | N   | CYS | 64 | 7.093  | -15.606 | -2.747 | 1.00 | 0.00 | 3A7 |
| ATOM | 163 | CA  | CYS | 64 | 7.601  | -16.598 | -3.674 | 1.00 | 0.00 | 3A7 |
| ATOM | 164 | CB  | CYS | 64 | 9.045  | -16.969 | -3.362 | 1.00 | 0.00 | 3A7 |
| ATOM | 165 | SG  | CYS | 64 | 9.973  | -15.524 | -3.736 | 1.00 | 0.00 | 3A7 |
| ATOM | 166 | C   | CYS | 64 | 6.805  | -17.853 | -3.631 | 1.00 | 0.00 | 3A7 |
| ATOM | 167 | O   | CYS | 64 | 6.413  | -18.402 | -4.655 | 1.00 | 0.00 | 3A7 |
| ATOM | 168 | N   | TYR | 65 | 6.477  | -18.323 | -2.413 | 1.00 | 0.00 | 3A7 |
| ATOM | 169 | CA  | TYR | 65 | 5.695  | -19.526 | -2.251 | 1.00 | 0.00 | 3A7 |
| ATOM | 170 | CB  | TYR | 65 | 5.638  | -19.993 | -0.802 | 1.00 | 0.00 | 3A7 |
| ATOM | 171 | CG  | TYR | 65 | 7.043  | -20.246 | -0.379 | 1.00 | 0.00 | 3A7 |
| ATOM | 172 | CD1 | TYR | 65 | 7.458  | -19.725 | 0.834  | 1.00 | 0.00 | 3A7 |

|      |     |     |     |    |        |         |         |      |      |     |
|------|-----|-----|-----|----|--------|---------|---------|------|------|-----|
| ATOM | 173 | CD2 | TYR | 65 | 7.985  | -20.850 | -1.222  | 1.00 | 0.00 | 3A7 |
| ATOM | 174 | CE1 | TYR | 65 | 8.800  | -19.750 | 1.182   | 1.00 | 0.00 | 3A7 |
| ATOM | 175 | CE2 | TYR | 65 | 9.336  | -20.816 | -0.901  | 1.00 | 0.00 | 3A7 |
| ATOM | 176 | CZ  | TYR | 65 | 9.743  | -20.216 | 0.283   | 1.00 | 0.00 | 3A7 |
| ATOM | 177 | OH  | TYR | 65 | 11.101 | -20.003 | 0.572   | 1.00 | 0.00 | 3A7 |
| ATOM | 178 | C   | TYR | 65 | 4.275  | -19.373 | -2.701  | 1.00 | 0.00 | 3A7 |
| ATOM | 179 | O   | TYR | 65 | 3.706  | -20.319 | -3.228  | 1.00 | 0.00 | 3A7 |
| ATOM | 180 | N   | LYS | 66 | 3.656  | -18.174 | -2.556  | 1.00 | 0.00 | 3A7 |
| ATOM | 181 | CA  | LYS | 66 | 2.313  | -17.922 | -3.043  | 1.00 | 0.00 | 3A7 |
| ATOM | 182 | CB  | LYS | 66 | 1.810  | -16.564 | -2.544  | 1.00 | 0.00 | 3A7 |
| ATOM | 183 | CG  | LYS | 66 | 1.450  | -16.579 | -1.049  | 1.00 | 0.00 | 3A7 |
| ATOM | 184 | CD  | LYS | 66 | 1.162  | -15.185 | -0.470  | 1.00 | 0.00 | 3A7 |
| ATOM | 185 | CE  | LYS | 66 | -0.063 | -14.502 | -1.089  | 1.00 | 0.00 | 3A7 |
| ATOM | 186 | NZ  | LYS | 66 | -0.299 | -13.182 | -0.461  | 1.00 | 0.00 | 3A7 |
| ATOM | 187 | C   | LYS | 66 | 2.244  | -17.957 | -4.556  | 1.00 | 0.00 | 3A7 |
| ATOM | 188 | O   | LYS | 66 | 1.227  | -18.326 | -5.129  | 1.00 | 0.00 | 3A7 |
| ATOM | 189 | N   | LYS | 67 | 3.349  | -17.595 | -5.243  | 1.00 | 0.00 | 3A7 |
| ATOM | 190 | CA  | LYS | 67 | 3.417  | -17.539 | -6.682  | 1.00 | 0.00 | 3A7 |
| ATOM | 191 | CB  | LYS | 67 | 4.377  | -16.414 | -7.137  | 1.00 | 0.00 | 3A7 |
| ATOM | 192 | CG  | LYS | 67 | 4.368  | -16.145 | -8.651  | 1.00 | 0.00 | 3A7 |
| ATOM | 193 | CD  | LYS | 67 | 5.148  | -14.878 | -9.034  | 1.00 | 0.00 | 3A7 |
| ATOM | 194 | CE  | LYS | 67 | 5.201  | -14.629 | -10.547 | 1.00 | 0.00 | 3A7 |
| ATOM | 195 | NZ  | LYS | 67 | 3.843  | -14.424 | -11.100 | 1.00 | 0.00 | 3A7 |
| ATOM | 196 | C   | LYS | 67 | 3.853  | -18.855 | -7.284  | 1.00 | 0.00 | 3A7 |
| ATOM | 197 | O   | LYS | 67 | 3.254  | -19.336 | -8.244  | 1.00 | 0.00 | 3A7 |
| ATOM | 198 | N   | TYR | 68 | 4.942  | -19.451 | -6.748  | 1.00 | 0.00 | 3A7 |
| ATOM | 199 | CA  | TYR | 68 | 5.626  | -20.573 | -7.355  | 1.00 | 0.00 | 3A7 |
| ATOM | 200 | CB  | TYR | 68 | 7.148  | -20.402 | -7.314  | 1.00 | 0.00 | 3A7 |
| ATOM | 201 | CG  | TYR | 68 | 7.522  | -19.259 | -8.216  | 1.00 | 0.00 | 3A7 |
| ATOM | 202 | CD1 | TYR | 68 | 7.789  | -17.989 | -7.702  | 1.00 | 0.00 | 3A7 |
| ATOM | 203 | CD2 | TYR | 68 | 7.593  | -19.457 | -9.595  | 1.00 | 0.00 | 3A7 |
| ATOM | 204 | CE1 | TYR | 68 | 8.122  | -16.937 | -8.550  | 1.00 | 0.00 | 3A7 |
| ATOM | 205 | CE2 | TYR | 68 | 7.927  | -18.408 | -10.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 206 | CZ  | TYR | 68 | 8.193  | -17.146 | -9.924  | 1.00 | 0.00 | 3A7 |
| ATOM | 207 | OH  | TYR | 68 | 8.537  | -16.080 | -10.784 | 1.00 | 0.00 | 3A7 |
| ATOM | 208 | C   | TYR | 68 | 5.236  | -21.899 | -6.770  | 1.00 | 0.00 | 3A7 |
| ATOM | 209 | O   | TYR | 68 | 5.299  | -22.918 | -7.453  | 1.00 | 0.00 | 3A7 |
| ATOM | 210 | N   | ARG | 69 | 4.785  | -21.912 | -5.500  | 1.00 | 0.00 | 3A7 |
| ATOM | 211 | CA  | ARG | 69 | 4.142  | -23.040 | -4.856  | 1.00 | 0.00 | 3A7 |
| ATOM | 212 | CB  | ARG | 69 | 3.046  | -23.733 | -5.717  | 1.00 | 0.00 | 3A7 |
| ATOM | 213 | CG  | ARG | 69 | 1.942  | -22.762 | -6.180  | 1.00 | 0.00 | 3A7 |
| ATOM | 214 | CD  | ARG | 69 | 0.844  | -23.441 | -7.009  | 1.00 | 0.00 | 3A7 |
| ATOM | 215 | NE  | ARG | 69 | 1.454  | -23.933 | -8.287  | 1.00 | 0.00 | 3A7 |
| ATOM | 216 | CZ  | ARG | 69 | 0.741  | -24.664 | -9.197  | 1.00 | 0.00 | 3A7 |
| ATOM | 217 | NH1 | ARG | 69 | 1.345  | -25.083 | -10.347 | 1.00 | 0.00 | 3A7 |
| ATOM | 218 | NH2 | ARG | 69 | -0.565 | -24.981 | -8.963  | 1.00 | 0.00 | 3A7 |
| ATOM | 219 | C   | ARG | 69 | 5.132  | -23.968 | -4.257  | 1.00 | 0.00 | 3A7 |
| ATOM | 220 | O   | ARG | 69 | 6.140  | -23.556 | -3.663  | 1.00 | 0.00 | 3A7 |
| ATOM | 221 | N   | LYS | 70 | 4.815  | -25.251 | -4.585  | 1.00 | 0.00 | 3A7 |
| ATOM | 222 | CA  | LYS | 70 | 5.551  | -26.459 | -4.410  | 1.00 | 0.00 | 3A7 |
| ATOM | 223 | CB  | LYS | 70 | 4.828  | -27.726 | -4.955  | 1.00 | 0.00 | 3A7 |
| ATOM | 224 | CG  | LYS | 70 | 3.527  | -28.142 | -4.233  | 1.00 | 0.00 | 3A7 |
| ATOM | 225 | CD  | LYS | 70 | 2.245  | -27.345 | -4.536  | 1.00 | 0.00 | 3A7 |
| ATOM | 226 | CE  | LYS | 70 | 1.635  | -27.577 | -5.929  | 1.00 | 0.00 | 3A7 |
| ATOM | 227 | NZ  | LYS | 70 | 2.449  | -26.976 | -7.009  | 1.00 | 0.00 | 3A7 |
| ATOM | 228 | C   | LYS | 70 | 6.866  | -26.352 | -5.122  | 1.00 | 0.00 | 3A7 |
| ATOM | 229 | O   | LYS | 70 | 7.015  | -26.860 | -6.233  | 1.00 | 0.00 | 3A7 |
| ATOM | 230 | N   | VAL | 71 | 7.834  | -25.662 | -4.449  | 1.00 | 0.00 | 3A7 |
| ATOM | 231 | CA  | VAL | 71 | 9.235  | -25.641 | -4.770  | 1.00 | 0.00 | 3A7 |
| ATOM | 232 | CB  | VAL | 71 | 9.760  | -26.967 | -5.362  | 1.00 | 0.00 | 3A7 |
| ATOM | 233 | CG1 | VAL | 71 | 11.270 | -26.882 | -5.635  | 1.00 | 0.00 | 3A7 |
| ATOM | 234 | CG2 | VAL | 71 | 9.523  | -28.158 | -4.411  | 1.00 | 0.00 | 3A7 |
| ATOM | 235 | C   | VAL | 71 | 9.454  | -24.472 | -5.708  | 1.00 | 0.00 | 3A7 |
| ATOM | 236 | O   | VAL | 71 | 8.810  | -24.376 | -6.751  | 1.00 | 0.00 | 3A7 |
| ATOM | 237 | N   | TRP | 72 | 10.373 | -23.545 | -5.337  | 1.00 | 0.00 | 3A7 |
| ATOM | 238 | CA  | TRP | 72 | 10.743 | -22.433 | -6.182  | 1.00 | 0.00 | 3A7 |
| ATOM | 239 | CB  | TRP | 72 | 10.009 | -21.089 | -5.839  | 1.00 | 0.00 | 3A7 |
| ATOM | 240 | CG  | TRP | 72 | 10.772 | -19.873 | -5.306  | 1.00 | 0.00 | 3A7 |
| ATOM | 241 | CD2 | TRP | 72 | 11.148 | -18.737 | -6.108  | 1.00 | 0.00 | 3A7 |
| ATOM | 242 | CD1 | TRP | 72 | 11.256 | -19.633 | -4.054  | 1.00 | 0.00 | 3A7 |
| ATOM | 243 | NE1 | TRP | 72 | 11.935 | -18.438 | -4.024  | 1.00 | 0.00 | 3A7 |
| ATOM | 244 | CE2 | TRP | 72 | 11.871 | -17.866 | -5.277  | 1.00 | 0.00 | 3A7 |



|      |     |     |     |    |        |         |         |      |      |     |
|------|-----|-----|-----|----|--------|---------|---------|------|------|-----|
| ATOM | 245 | CE3 | TRP | 72 | 10.923 | -18.434 | -7.436  | 1.00 | 0.00 | 3A7 |
| ATOM | 246 | CZ2 | TRP | 72 | 12.368 | -16.672 | -5.760  | 1.00 | 0.00 | 3A7 |
| ATOM | 247 | CZ3 | TRP | 72 | 11.414 | -17.223 | -7.920  | 1.00 | 0.00 | 3A7 |
| ATOM | 248 | CH2 | TRP | 72 | 12.124 | -16.354 | -7.094  | 1.00 | 0.00 | 3A7 |
| ATOM | 249 | C   | TRP | 72 | 12.229 | -22.293 | -6.064  | 1.00 | 0.00 | 3A7 |
| ATOM | 250 | O   | TRP | 72 | 12.824 | -22.782 | -5.112  | 1.00 | 0.00 | 3A7 |
| ATOM | 251 | N   | GLY | 73 | 12.861 | -21.582 | -7.022  | 1.00 | 0.00 | 3A7 |
| ATOM | 252 | CA  | GLY | 73 | 14.278 | -21.323 | -6.985  | 1.00 | 0.00 | 3A7 |
| ATOM | 253 | C   | GLY | 73 | 14.511 | -19.850 | -6.821  | 1.00 | 0.00 | 3A7 |
| ATOM | 254 | O   | GLY | 73 | 13.812 | -19.031 | -7.409  | 1.00 | 0.00 | 3A7 |
| ATOM | 255 | N   | ILE | 74 | 15.530 | -19.484 | -6.009  | 1.00 | 0.00 | 3A7 |
| ATOM | 256 | CA  | ILE | 74 | 15.929 | -18.120 | -5.754  | 1.00 | 0.00 | 3A7 |
| ATOM | 257 | CB  | ILE | 74 | 15.600 | -17.676 | -4.328  | 1.00 | 0.00 | 3A7 |
| ATOM | 258 | CG2 | ILE | 74 | 16.301 | -18.543 | -3.258  | 1.00 | 0.00 | 3A7 |
| ATOM | 259 | CG1 | ILE | 74 | 15.835 | -16.159 | -4.124  | 1.00 | 0.00 | 3A7 |
| ATOM | 260 | CD  | ILE | 74 | 15.205 | -15.621 | -2.836  | 1.00 | 0.00 | 3A7 |
| ATOM | 261 | C   | ILE | 74 | 17.407 | -18.077 | -6.023  | 1.00 | 0.00 | 3A7 |
| ATOM | 262 | O   | ILE | 74 | 18.100 | -19.082 | -5.904  | 1.00 | 0.00 | 3A7 |
| ATOM | 263 | N   | TYR | 75 | 17.928 | -16.900 | -6.425  | 1.00 | 0.00 | 3A7 |
| ATOM | 264 | CA  | TYR | 75 | 19.303 | -16.765 | -6.827  | 1.00 | 0.00 | 3A7 |
| ATOM | 265 | CB  | TYR | 75 | 19.424 | -16.348 | -8.308  | 1.00 | 0.00 | 3A7 |
| ATOM | 266 | CG  | TYR | 75 | 18.811 | -17.400 | -9.184  | 1.00 | 0.00 | 3A7 |
| ATOM | 267 | CD1 | TYR | 75 | 17.487 | -17.281 | -9.613  | 1.00 | 0.00 | 3A7 |
| ATOM | 268 | CD2 | TYR | 75 | 19.554 | -18.513 | -9.582  | 1.00 | 0.00 | 3A7 |
| ATOM | 269 | CE1 | TYR | 75 | 16.911 | -18.261 | -10.415 | 1.00 | 0.00 | 3A7 |
| ATOM | 270 | CE2 | TYR | 75 | 18.983 | -19.489 | -10.394 | 1.00 | 0.00 | 3A7 |
| ATOM | 271 | CZ  | TYR | 75 | 17.660 | -19.367 | -10.807 | 1.00 | 0.00 | 3A7 |
| ATOM | 272 | OH  | TYR | 75 | 17.079 | -20.361 | -11.624 | 1.00 | 0.00 | 3A7 |
| ATOM | 273 | C   | TYR | 75 | 19.927 | -15.716 | -5.954  | 1.00 | 0.00 | 3A7 |
| ATOM | 274 | O   | TYR | 75 | 19.589 | -14.543 | -6.059  | 1.00 | 0.00 | 3A7 |
| ATOM | 275 | N   | ASP | 76 | 20.867 | -16.106 | -5.059  | 1.00 | 0.00 | 3A7 |
| ATOM | 276 | CA  | ASP | 76 | 21.559 | -15.171 | -4.194  | 1.00 | 0.00 | 3A7 |
| ATOM | 277 | CB  | ASP | 76 | 21.470 | -15.513 | -2.685  | 1.00 | 0.00 | 3A7 |
| ATOM | 278 | CG  | ASP | 76 | 20.053 | -15.259 | -2.172  | 1.00 | 0.00 | 3A7 |
| ATOM | 279 | OD1 | ASP | 76 | 19.105 | -15.935 | -2.652  | 1.00 | 0.00 | 3A7 |
| ATOM | 280 | OD2 | ASP | 76 | 19.905 | -14.382 | -1.279  | 1.00 | 0.00 | 3A7 |
| ATOM | 281 | C   | ASP | 76 | 23.004 | -15.175 | -4.597  | 1.00 | 0.00 | 3A7 |
| ATOM | 282 | O   | ASP | 76 | 23.790 | -16.000 | -4.149  | 1.00 | 0.00 | 3A7 |
| ATOM | 283 | N   | CYS | 77 | 23.393 | -14.210 | -5.459  | 1.00 | 0.00 | 3A7 |
| ATOM | 284 | CA  | CYS | 77 | 24.738 | -13.896 | -5.902  | 1.00 | 0.00 | 3A7 |
| ATOM | 285 | CB  | CYS | 77 | 25.569 | -13.074 | -4.858  | 1.00 | 0.00 | 3A7 |
| ATOM | 286 | SG  | CYS | 77 | 25.906 | -13.854 | -3.237  | 1.00 | 0.00 | 3A7 |
| ATOM | 287 | C   | CYS | 77 | 25.544 | -15.056 | -6.442  | 1.00 | 0.00 | 3A7 |
| ATOM | 288 | O   | CYS | 77 | 26.561 | -15.442 | -5.879  | 1.00 | 0.00 | 3A7 |
| ATOM | 289 | N   | GLN | 78 | 25.091 | -15.613 | -7.583  | 1.00 | 0.00 | 3A7 |
| ATOM | 290 | CA  | GLN | 78 | 25.770 | -16.622 | -8.369  | 1.00 | 0.00 | 3A7 |
| ATOM | 291 | CB  | GLN | 78 | 27.325 | -16.549 | -8.440  | 1.00 | 0.00 | 3A7 |
| ATOM | 292 | CG  | GLN | 78 | 27.848 | -15.222 | -9.017  | 1.00 | 0.00 | 3A7 |
| ATOM | 293 | CD  | GLN | 78 | 29.378 | -15.274 | -9.063  | 1.00 | 0.00 | 3A7 |
| ATOM | 294 | OE1 | GLN | 78 | 29.961 | -16.057 | -9.823  | 1.00 | 0.00 | 3A7 |
| ATOM | 295 | NE2 | GLN | 78 | 30.031 | -14.415 | -8.222  | 1.00 | 0.00 | 3A7 |
| ATOM | 296 | C   | GLN | 78 | 25.375 | -18.037 | -8.023  | 1.00 | 0.00 | 3A7 |
| ATOM | 297 | O   | GLN | 78 | 25.715 | -18.949 | -8.771  | 1.00 | 0.00 | 3A7 |
| ATOM | 298 | N   | GLN | 79 | 24.653 | -18.277 | -6.903  | 1.00 | 0.00 | 3A7 |
| ATOM | 299 | CA  | GLN | 79 | 24.270 | -19.620 | -6.516  | 1.00 | 0.00 | 3A7 |
| ATOM | 300 | CB  | GLN | 79 | 24.718 | -19.978 | -5.085  | 1.00 | 0.00 | 3A7 |
| ATOM | 301 | CG  | GLN | 79 | 26.242 | -19.895 | -4.897  | 1.00 | 0.00 | 3A7 |
| ATOM | 302 | CD  | GLN | 79 | 26.582 | -20.276 | -3.453  | 1.00 | 0.00 | 3A7 |
| ATOM | 303 | OE1 | GLN | 79 | 26.176 | -19.589 | -2.508  | 1.00 | 0.00 | 3A7 |
| ATOM | 304 | NE2 | GLN | 79 | 27.346 | -21.399 | -3.294  | 1.00 | 0.00 | 3A7 |
| ATOM | 305 | C   | GLN | 79 | 22.765 | -19.774 | -6.615  | 1.00 | 0.00 | 3A7 |
| ATOM | 306 | O   | GLN | 79 | 22.037 | -18.847 | -6.260  | 1.00 | 0.00 | 3A7 |
| ATOM | 307 | N   | PRO | 80 | 22.241 | -20.926 | -7.069  | 1.00 | 0.00 | 3A7 |
| ATOM | 308 | CA  | PRO | 80 | 20.824 | -21.225 | -7.042  | 1.00 | 0.00 | 3A7 |
| ATOM | 309 | CD  | PRO | 80 | 22.976 | -21.867 | -7.907  | 1.00 | 0.00 | 3A7 |
| ATOM | 310 | CB  | PRO | 80 | 20.605 | -22.191 | -8.214  | 1.00 | 0.00 | 3A7 |
| ATOM | 311 | CG  | PRO | 80 | 21.950 | -22.915 | -8.360  | 1.00 | 0.00 | 3A7 |
| ATOM | 312 | C   | PRO | 80 | 20.502 | -21.899 | -5.737  | 1.00 | 0.00 | 3A7 |
| ATOM | 313 | O   | PRO | 80 | 21.269 | -22.746 | -5.277  | 1.00 | 0.00 | 3A7 |
| ATOM | 314 | N   | MET | 81 | 19.342 | -21.571 | -5.140  | 1.00 | 0.00 | 3A7 |
| ATOM | 315 | CA  | MET | 81 | 18.883 | -22.233 | -3.952  | 1.00 | 0.00 | 3A7 |
| ATOM | 316 | CB  | MET | 81 | 19.098 | -21.392 | -2.669  | 1.00 | 0.00 | 3A7 |

|      |     |     |     |    |        |         |        |      |      |     |
|------|-----|-----|-----|----|--------|---------|--------|------|------|-----|
| ATOM | 317 | CG  | MET | 81 | 20.582 | -21.043 | -2.428 | 1.00 | 0.00 | 3A7 |
| ATOM | 318 | SD  | MET | 81 | 20.947 | -20.209 | -0.854 | 1.00 | 0.00 | 3A7 |
| ATOM | 319 | CE  | MET | 81 | 20.120 | -18.650 | -1.276 | 1.00 | 0.00 | 3A7 |
| ATOM | 320 | C   | MET | 81 | 17.447 | -22.487 | -4.177 | 1.00 | 0.00 | 3A7 |
| ATOM | 321 | O   | MET | 81 | 16.677 | -21.572 | -4.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 322 | N   | LEU | 82 | 17.035 | -23.763 | -4.052 | 1.00 | 0.00 | 3A7 |
| ATOM | 323 | CA  | LEU | 82 | 15.657 | -24.130 | -4.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 324 | CB  | LEU | 82 | 15.468 | -25.434 | -4.990 | 1.00 | 0.00 | 3A7 |
| ATOM | 325 | CG  | LEU | 82 | 15.574 | -25.122 | -6.509 | 1.00 | 0.00 | 3A7 |
| ATOM | 326 | CD1 | LEU | 82 | 16.903 | -25.569 | -7.137 | 1.00 | 0.00 | 3A7 |
| ATOM | 327 | CD2 | LEU | 82 | 14.352 | -25.622 | -7.300 | 1.00 | 0.00 | 3A7 |
| ATOM | 328 | C   | LEU | 82 | 15.022 | -24.179 | -2.843 | 1.00 | 0.00 | 3A7 |
| ATOM | 329 | O   | LEU | 82 | 15.439 | -24.903 | -1.947 | 1.00 | 0.00 | 3A7 |
| ATOM | 330 | N   | ALA | 83 | 13.975 | -23.351 | -2.673 | 1.00 | 0.00 | 3A7 |
| ATOM | 331 | CA  | ALA | 83 | 13.243 | -23.210 | -1.443 | 1.00 | 0.00 | 3A7 |
| ATOM | 332 | CB  | ALA | 83 | 12.731 | -21.792 | -1.267 | 1.00 | 0.00 | 3A7 |
| ATOM | 333 | C   | ALA | 83 | 12.040 | -24.096 | -1.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 334 | O   | ALA | 83 | 11.193 | -24.025 | -2.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 335 | N   | ILE | 84 | 11.963 | -24.967 | -0.399 | 1.00 | 0.00 | 3A7 |
| ATOM | 336 | CA  | ILE | 84 | 10.949 | -25.985 | -0.290 | 1.00 | 0.00 | 3A7 |
| ATOM | 337 | CB  | ILE | 84 | 11.517 | -27.364 | 0.009  | 1.00 | 0.00 | 3A7 |
| ATOM | 338 | CG2 | ILE | 84 | 10.376 | -28.307 | 0.374  | 1.00 | 0.00 | 3A7 |
| ATOM | 339 | CG1 | ILE | 84 | 12.173 | -28.016 | -1.243 | 1.00 | 0.00 | 3A7 |
| ATOM | 340 | CD  | ILE | 84 | 13.207 | -27.201 | -2.013 | 1.00 | 0.00 | 3A7 |
| ATOM | 341 | C   | ILE | 84 | 10.004 | -25.576 | 0.802  | 1.00 | 0.00 | 3A7 |
| ATOM | 342 | O   | ILE | 84 | 10.404 | -25.289 | 1.921  | 1.00 | 0.00 | 3A7 |
| ATOM | 343 | N   | THR | 85 | 8.689  | -25.597 | 0.509  | 1.00 | 0.00 | 3A7 |
| ATOM | 344 | CA  | THR | 85 | 7.672  | -25.139 | 1.413  | 1.00 | 0.00 | 3A7 |
| ATOM | 345 | CB  | THR | 85 | 7.073  | -23.819 | 0.999  | 1.00 | 0.00 | 3A7 |
| ATOM | 346 | OG1 | THR | 85 | 7.093  | -23.627 | -0.412 | 1.00 | 0.00 | 3A7 |
| ATOM | 347 | CG2 | THR | 85 | 7.922  | -22.782 | 1.725  | 1.00 | 0.00 | 3A7 |
| ATOM | 348 | C   | THR | 85 | 6.562  | -26.125 | 1.486  | 1.00 | 0.00 | 3A7 |
| ATOM | 349 | O   | THR | 85 | 6.050  | -26.730 | 0.619  | 1.00 | 0.00 | 3A7 |
| ATOM | 350 | N   | ASP | 86 | 5.995  | -26.396 | 2.502  | 1.00 | 0.00 | 3A7 |
| ATOM | 351 | CA  | ASP | 86 | 4.810  | -27.263 | 2.510  | 1.00 | 0.00 | 3A7 |
| ATOM | 352 | CB  | ASP | 86 | 3.722  | -27.421 | 1.361  | 1.00 | 0.00 | 3A7 |
| ATOM | 353 | CG  | ASP | 86 | 3.168  | -26.055 | 0.952  | 1.00 | 0.00 | 3A7 |
| ATOM | 354 | OD1 | ASP | 86 | 2.591  | -25.362 | 1.833  | 1.00 | 0.00 | 3A7 |
| ATOM | 355 | OD2 | ASP | 86 | 3.312  | -25.692 | -0.246 | 1.00 | 0.00 | 3A7 |
| ATOM | 356 | C   | ASP | 86 | 5.268  | -28.602 | 3.011  | 1.00 | 0.00 | 3A7 |
| ATOM | 357 | O   | ASP | 86 | 6.399  | -28.994 | 2.738  | 1.00 | 0.00 | 3A7 |
| ATOM | 358 | N   | PRO | 87 | 4.433  | -29.324 | 3.756  | 1.00 | 0.00 | 3A7 |
| ATOM | 359 | CA  | PRO | 87 | 4.827  | -30.519 | 4.472  | 1.00 | 0.00 | 3A7 |
| ATOM | 360 | CD  | PRO | 87 | 3.262  | -28.734 | 4.388  | 1.00 | 0.00 | 3A7 |
| ATOM | 361 | CB  | PRO | 87 | 3.599  | -30.942 | 5.276  | 1.00 | 0.00 | 3A7 |
| ATOM | 362 | CG  | PRO | 87 | 2.505  | -29.914 | 4.977  | 1.00 | 0.00 | 3A7 |
| ATOM | 363 | C   | PRO | 87 | 5.202  | -31.641 | 3.571  | 1.00 | 0.00 | 3A7 |
| ATOM | 364 | O   | PRO | 87 | 6.112  | -32.375 | 3.920  | 1.00 | 0.00 | 3A7 |
| ATOM | 365 | N   | ASP | 88 | 4.533  | -31.800 | 2.413  | 1.00 | 0.00 | 3A7 |
| ATOM | 366 | CA  | ASP | 88 | 4.791  | -32.846 | 1.455  | 1.00 | 0.00 | 3A7 |
| ATOM | 367 | CB  | ASP | 88 | 3.829  | -32.701 | 0.270  | 1.00 | 0.00 | 3A7 |
| ATOM | 368 | CG  | ASP | 88 | 2.381  | -32.826 | 0.749  | 1.00 | 0.00 | 3A7 |
| ATOM | 369 | OD1 | ASP | 88 | 2.122  | -33.640 | 1.676  | 1.00 | 0.00 | 3A7 |
| ATOM | 370 | OD2 | ASP | 88 | 1.516  | -32.094 | 0.198  | 1.00 | 0.00 | 3A7 |
| ATOM | 371 | C   | ASP | 88 | 6.196  | -32.787 | 0.909  | 1.00 | 0.00 | 3A7 |
| ATOM | 372 | O   | ASP | 88 | 6.874  | -33.798 | 0.830  | 1.00 | 0.00 | 3A7 |
| ATOM | 373 | N   | MET | 89 | 6.691  | -31.588 | 0.554  | 1.00 | 0.00 | 3A7 |
| ATOM | 374 | CA  | MET | 89 | 8.014  | -31.388 | 0.009  | 1.00 | 0.00 | 3A7 |
| ATOM | 375 | CB  | MET | 89 | 8.081  | -30.073 | -0.773 | 1.00 | 0.00 | 3A7 |
| ATOM | 376 | CG  | MET | 89 | 7.065  | -30.035 | -1.918 | 1.00 | 0.00 | 3A7 |
| ATOM | 377 | SD  | MET | 89 | 5.914  | -28.663 | -1.731 | 1.00 | 0.00 | 3A7 |
| ATOM | 378 | CE  | MET | 89 | 7.247  | -27.425 | -1.755 | 1.00 | 0.00 | 3A7 |
| ATOM | 379 | C   | MET | 89 | 9.069  | -31.390 | 1.081  | 1.00 | 0.00 | 3A7 |
| ATOM | 380 | O   | MET | 89 | 10.152 | -31.936 | 0.893  | 1.00 | 0.00 | 3A7 |
| ATOM | 381 | N   | ILE | 90 | 8.754  | -30.824 | 2.267  | 1.00 | 0.00 | 3A7 |
| ATOM | 382 | CA  | ILE | 90 | 9.657  | -30.812 | 3.398  | 1.00 | 0.00 | 3A7 |
| ATOM | 383 | CB  | ILE | 90 | 9.126  | -29.908 | 4.501  | 1.00 | 0.00 | 3A7 |
| ATOM | 384 | CG2 | ILE | 90 | 9.952  | -30.036 | 5.807  | 1.00 | 0.00 | 3A7 |
| ATOM | 385 | CG1 | ILE | 90 | 9.060  | -28.467 | 3.973  | 1.00 | 0.00 | 3A7 |
| ATOM | 386 | CD  | ILE | 90 | 10.436 | -27.853 | 3.815  | 1.00 | 0.00 | 3A7 |
| ATOM | 387 | C   | ILE | 90 | 9.898  | -32.218 | 3.920  | 1.00 | 0.00 | 3A7 |
| ATOM | 388 | O   | ILE | 90 | 11.016 | -32.588 | 4.248  | 1.00 | 0.00 | 3A7 |

|      |     |     |     |    |        |         |        |      |      |     |
|------|-----|-----|-----|----|--------|---------|--------|------|------|-----|
| ATOM | 389 | N   | LYS | 91 | 8.877  | -33.100 | 3.925  | 1.00 | 0.00 | 3A7 |
| ATOM | 390 | CA  | LYS | 91 | 9.058  | -34.479 | 4.328  | 1.00 | 0.00 | 3A7 |
| ATOM | 391 | CB  | LYS | 91 | 7.722  | -35.240 | 4.361  | 1.00 | 0.00 | 3A7 |
| ATOM | 392 | CG  | LYS | 91 | 7.790  | -36.619 | 5.036  | 1.00 | 0.00 | 3A7 |
| ATOM | 393 | CD  | LYS | 91 | 6.407  | -37.269 | 5.192  | 1.00 | 0.00 | 3A7 |
| ATOM | 394 | CE  | LYS | 91 | 6.465  | -38.628 | 5.898  | 1.00 | 0.00 | 3A7 |
| ATOM | 395 | NZ  | LYS | 91 | 5.108  | -39.206 | 6.031  | 1.00 | 0.00 | 3A7 |
| ATOM | 396 | C   | LYS | 91 | 10.010 | -35.209 | 3.414  | 1.00 | 0.00 | 3A7 |
| ATOM | 397 | O   | LYS | 91 | 10.824 | -36.021 | 3.838  | 1.00 | 0.00 | 3A7 |
| ATOM | 398 | N   | THR | 92 | 9.969  | -34.861 | 2.113  | 1.00 | 0.00 | 3A7 |
| ATOM | 399 | CA  | THR | 92 | 10.864 | -35.382 | 1.113  | 1.00 | 0.00 | 3A7 |
| ATOM | 400 | CB  | THR | 92 | 10.441 | -34.980 | -0.272 | 1.00 | 0.00 | 3A7 |
| ATOM | 401 | OG1 | THR | 92 | 9.047  | -35.206 | -0.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 402 | CG2 | THR | 92 | 11.180 | -35.836 | -1.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 403 | C   | THR | 92 | 12.263 | -34.904 | 1.326  | 1.00 | 0.00 | 3A7 |
| ATOM | 404 | O   | THR | 92 | 13.222 | -35.657 | 1.196  | 1.00 | 0.00 | 3A7 |
| ATOM | 405 | N   | VAL | 93 | 12.395 | -33.620 | 1.730  | 1.00 | 0.00 | 3A7 |
| ATOM | 406 | CA  | VAL | 93 | 13.674 | -33.006 | 1.938  | 1.00 | 0.00 | 3A7 |
| ATOM | 407 | CB  | VAL | 93 | 13.628 | -31.500 | 2.127  | 1.00 | 0.00 | 3A7 |
| ATOM | 408 | CG1 | VAL | 93 | 12.833 | -30.752 | 1.061  | 1.00 | 0.00 | 3A7 |
| ATOM | 409 | CG2 | VAL | 93 | 13.354 | -31.074 | 3.585  | 1.00 | 0.00 | 3A7 |
| ATOM | 410 | C   | VAL | 93 | 14.483 | -33.705 | 3.034  | 1.00 | 0.00 | 3A7 |
| ATOM | 411 | O   | VAL | 93 | 15.703 | -33.627 | 3.002  | 1.00 | 0.00 | 3A7 |
| ATOM | 412 | N   | LEU | 94 | 13.861 | -34.522 | 3.946  | 1.00 | 0.00 | 3A7 |
| ATOM | 413 | CA  | LEU | 94 | 14.509 | -35.450 | 4.889  | 1.00 | 0.00 | 3A7 |
| ATOM | 414 | CB  | LEU | 94 | 13.538 | -36.540 | 5.429  | 1.00 | 0.00 | 3A7 |
| ATOM | 415 | CG  | LEU | 94 | 12.454 | -36.028 | 6.397  | 1.00 | 0.00 | 3A7 |
| ATOM | 416 | CD1 | LEU | 94 | 11.435 | -37.136 | 6.726  | 1.00 | 0.00 | 3A7 |
| ATOM | 417 | CD2 | LEU | 94 | 13.079 | -35.489 | 7.687  | 1.00 | 0.00 | 3A7 |
| ATOM | 418 | C   | LEU | 94 | 15.673 | -36.253 | 4.325  | 1.00 | 0.00 | 3A7 |
| ATOM | 419 | O   | LEU | 94 | 16.786 | -36.171 | 4.842  | 1.00 | 0.00 | 3A7 |
| ATOM | 420 | N   | VAL | 95 | 15.389 | -37.041 | 3.249  | 1.00 | 0.00 | 3A7 |
| ATOM | 421 | CA  | VAL | 95 | 16.254 | -37.904 | 2.446  | 1.00 | 0.00 | 3A7 |
| ATOM | 422 | CB  | VAL | 95 | 17.146 | -37.147 | 1.449  | 1.00 | 0.00 | 3A7 |
| ATOM | 423 | CG1 | VAL | 95 | 18.293 | -36.331 | 2.088  | 1.00 | 0.00 | 3A7 |
| ATOM | 424 | CG2 | VAL | 95 | 17.667 | -38.131 | 0.379  | 1.00 | 0.00 | 3A7 |
| ATOM | 425 | C   | VAL | 95 | 17.019 | -38.932 | 3.269  | 1.00 | 0.00 | 3A7 |
| ATOM | 426 | O   | VAL | 95 | 17.910 | -38.606 | 4.052  | 1.00 | 0.00 | 3A7 |
| ATOM | 427 | N   | LYS | 96 | 16.651 | -40.226 | 3.099  | 1.00 | 0.00 | 3A7 |
| ATOM | 428 | CA  | LYS | 96 | 17.216 | -41.310 | 3.864  | 1.00 | 0.00 | 3A7 |
| ATOM | 429 | CB  | LYS | 96 | 16.284 | -41.757 | 5.021  | 1.00 | 0.00 | 3A7 |
| ATOM | 430 | CG  | LYS | 96 | 16.863 | -42.863 | 5.922  | 1.00 | 0.00 | 3A7 |
| ATOM | 431 | CD  | LYS | 96 | 15.917 | -43.296 | 7.055  | 1.00 | 0.00 | 3A7 |
| ATOM | 432 | CE  | LYS | 96 | 15.646 | -42.211 | 8.105  | 1.00 | 0.00 | 3A7 |
| ATOM | 433 | NZ  | LYS | 96 | 16.899 | -41.808 | 8.783  | 1.00 | 0.00 | 3A7 |
| ATOM | 434 | C   | LYS | 96 | 17.438 | -42.463 | 2.917  | 1.00 | 0.00 | 3A7 |
| ATOM | 435 | O   | LYS | 96 | 16.460 | -42.998 | 2.397  | 1.00 | 0.00 | 3A7 |
| ATOM | 436 | N   | GLU | 97 | 18.697 | -42.930 | 2.649  | 1.00 | 0.00 | 3A7 |
| ATOM | 437 | CA  | GLU | 97 | 20.025 | -42.451 | 3.016  | 1.00 | 0.00 | 3A7 |
| ATOM | 438 | CB  | GLU | 97 | 20.351 | -41.024 | 2.498  | 1.00 | 0.00 | 3A7 |
| ATOM | 439 | CG  | GLU | 97 | 20.271 | -40.894 | 0.966  | 1.00 | 0.00 | 3A7 |
| ATOM | 440 | CD  | GLU | 97 | 21.342 | -41.763 | 0.314  | 1.00 | 0.00 | 3A7 |
| ATOM | 441 | OE1 | GLU | 97 | 20.968 | -42.695 | -0.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 442 | OE2 | GLU | 97 | 22.549 | -41.504 | 0.567  | 1.00 | 0.00 | 3A7 |
| ATOM | 443 | C   | GLU | 97 | 20.318 | -42.531 | 4.499  | 1.00 | 0.00 | 3A7 |
| ATOM | 444 | O   | GLU | 97 | 20.158 | -41.560 | 5.238  | 1.00 | 0.00 | 3A7 |
| ATOM | 445 | N   | CYS | 98 | 20.813 | -43.711 | 4.956  | 1.00 | 0.00 | 3A7 |
| ATOM | 446 | CA  | CYS | 98 | 21.223 | -43.956 | 6.327  | 1.00 | 0.00 | 3A7 |
| ATOM | 447 | CB  | CYS | 98 | 21.159 | -45.456 | 6.703  | 1.00 | 0.00 | 3A7 |
| ATOM | 448 | SG  | CYS | 98 | 19.470 | -46.111 | 6.530  | 1.00 | 0.00 | 3A7 |
| ATOM | 449 | C   | CYS | 98 | 22.633 | -43.454 | 6.538  | 1.00 | 0.00 | 3A7 |
| ATOM | 450 | O   | CYS | 98 | 23.032 | -43.131 | 7.656  | 1.00 | 0.00 | 3A7 |
| ATOM | 451 | N   | TYR | 99 | 23.399 | -43.358 | 5.423  | 1.00 | 0.00 | 3A7 |
| ATOM | 452 | CA  | TYR | 99 | 24.680 | -42.699 | 5.352  | 1.00 | 0.00 | 3A7 |
| ATOM | 453 | CB  | TYR | 99 | 25.794 | -43.602 | 4.775  | 1.00 | 0.00 | 3A7 |
| ATOM | 454 | CG  | TYR | 99 | 26.067 | -44.708 | 5.749  | 1.00 | 0.00 | 3A7 |
| ATOM | 455 | CD1 | TYR | 99 | 25.528 | -45.981 | 5.553  | 1.00 | 0.00 | 3A7 |
| ATOM | 456 | CD2 | TYR | 99 | 26.855 | -44.471 | 6.875  | 1.00 | 0.00 | 3A7 |
| ATOM | 457 | CE1 | TYR | 99 | 25.771 | -47.000 | 6.470  | 1.00 | 0.00 | 3A7 |
| ATOM | 458 | CE2 | TYR | 99 | 27.103 | -45.488 | 7.791  | 1.00 | 0.00 | 3A7 |
| ATOM | 459 | CZ  | TYR | 99 | 26.560 | -46.754 | 7.591  | 1.00 | 0.00 | 3A7 |
| ATOM | 460 | OH  | TYR | 99 | 26.807 | -47.785 | 8.524  | 1.00 | 0.00 | 3A7 |

|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 461 | C   | TYR | 99  | 24.459 | -41.520 | 4.445  | 1.00 | 0.00 | 3A7 |
| ATOM | 462 | O   | TYR | 99  | 24.717 | -41.584 | 3.244  | 1.00 | 0.00 | 3A7 |
| ATOM | 463 | N   | SER | 100 | 23.943 | -40.407 | 5.029  | 1.00 | 0.00 | 3A7 |
| ATOM | 464 | CA  | SER | 100 | 23.548 | -39.211 | 4.317  | 1.00 | 0.00 | 3A7 |
| ATOM | 465 | CB  | SER | 100 | 22.340 | -38.501 | 4.990  | 1.00 | 0.00 | 3A7 |
| ATOM | 466 | OG  | SER | 100 | 22.547 | -38.275 | 6.381  | 1.00 | 0.00 | 3A7 |
| ATOM | 467 | C   | SER | 100 | 24.721 | -38.267 | 4.207  | 1.00 | 0.00 | 3A7 |
| ATOM | 468 | O   | SER | 100 | 25.295 | -37.848 | 5.211  | 1.00 | 0.00 | 3A7 |
| ATOM | 469 | N   | VAL | 101 | 25.093 | -37.923 | 2.947  | 1.00 | 0.00 | 3A7 |
| ATOM | 470 | CA  | VAL | 101 | 26.233 | -37.096 | 2.616  | 1.00 | 0.00 | 3A7 |
| ATOM | 471 | CB  | VAL | 101 | 26.925 | -37.529 | 1.327  | 1.00 | 0.00 | 3A7 |
| ATOM | 472 | CG1 | VAL | 101 | 28.244 | -36.746 | 1.143  | 1.00 | 0.00 | 3A7 |
| ATOM | 473 | CG2 | VAL | 101 | 27.188 | -39.049 | 1.394  | 1.00 | 0.00 | 3A7 |
| ATOM | 474 | C   | VAL | 101 | 25.777 | -35.663 | 2.512  | 1.00 | 0.00 | 3A7 |
| ATOM | 475 | O   | VAL | 101 | 25.384 | -35.187 | 1.447  | 1.00 | 0.00 | 3A7 |
| ATOM | 476 | N   | PHE | 102 | 25.851 | -34.944 | 3.658  | 1.00 | 0.00 | 3A7 |
| ATOM | 477 | CA  | PHE | 102 | 25.588 | -33.531 | 3.774  | 1.00 | 0.00 | 3A7 |
| ATOM | 478 | CB  | PHE | 102 | 24.757 | -33.208 | 5.051  | 1.00 | 0.00 | 3A7 |
| ATOM | 479 | CG  | PHE | 102 | 24.515 | -31.734 | 5.284  | 1.00 | 0.00 | 3A7 |
| ATOM | 480 | CD1 | PHE | 102 | 24.224 | -30.854 | 4.236  | 1.00 | 0.00 | 3A7 |
| ATOM | 481 | CD2 | PHE | 102 | 24.602 | -31.227 | 6.582  | 1.00 | 0.00 | 3A7 |
| ATOM | 482 | CE1 | PHE | 102 | 24.063 | -29.493 | 4.481  | 1.00 | 0.00 | 3A7 |
| ATOM | 483 | CE2 | PHE | 102 | 24.424 | -29.870 | 6.830  | 1.00 | 0.00 | 3A7 |
| ATOM | 484 | CZ  | PHE | 102 | 24.163 | -29.000 | 5.777  | 1.00 | 0.00 | 3A7 |
| ATOM | 485 | C   | PHE | 102 | 26.945 | -32.887 | 3.838  | 1.00 | 0.00 | 3A7 |
| ATOM | 486 | O   | PHE | 102 | 27.728 | -33.174 | 4.741  | 1.00 | 0.00 | 3A7 |
| ATOM | 487 | N   | THR | 103 | 27.238 | -31.980 | 2.869  | 1.00 | 0.00 | 3A7 |
| ATOM | 488 | CA  | THR | 103 | 28.502 | -31.281 | 2.757  | 1.00 | 0.00 | 3A7 |
| ATOM | 489 | CB  | THR | 103 | 28.814 | -30.904 | 1.308  | 1.00 | 0.00 | 3A7 |
| ATOM | 490 | OG1 | THR | 103 | 30.168 | -30.496 | 1.135  | 1.00 | 0.00 | 3A7 |
| ATOM | 491 | CG2 | THR | 103 | 27.858 | -29.816 | 0.779  | 1.00 | 0.00 | 3A7 |
| ATOM | 492 | C   | THR | 103 | 28.484 | -30.083 | 3.685  | 1.00 | 0.00 | 3A7 |
| ATOM | 493 | O   | THR | 103 | 27.430 | -29.672 | 4.169  | 1.00 | 0.00 | 3A7 |
| ATOM | 494 | N   | ASN | 104 | 29.682 | -29.507 | 3.955  | 1.00 | 0.00 | 3A7 |
| ATOM | 495 | CA  | ASN | 104 | 29.888 | -28.430 | 4.899  | 1.00 | 0.00 | 3A7 |
| ATOM | 496 | CB  | ASN | 104 | 31.378 | -28.320 | 5.343  | 1.00 | 0.00 | 3A7 |
| ATOM | 497 | CG  | ASN | 104 | 32.353 | -28.168 | 4.161  | 1.00 | 0.00 | 3A7 |
| ATOM | 498 | OD1 | ASN | 104 | 32.706 | -27.047 | 3.775  | 1.00 | 0.00 | 3A7 |
| ATOM | 499 | ND2 | ASN | 104 | 32.796 | -29.333 | 3.597  | 1.00 | 0.00 | 3A7 |
| ATOM | 500 | C   | ASN | 104 | 29.418 | -27.105 | 4.342  | 1.00 | 0.00 | 3A7 |
| ATOM | 501 | O   | ASN | 104 | 29.471 | -26.868 | 3.135  | 1.00 | 0.00 | 3A7 |
| ATOM | 502 | N   | ARG | 105 | 28.961 | -26.205 | 5.250  | 1.00 | 0.00 | 3A7 |
| ATOM | 503 | CA  | ARG | 105 | 28.538 | -24.859 | 4.929  | 1.00 | 0.00 | 3A7 |
| ATOM | 504 | CB  | ARG | 105 | 27.556 | -24.275 | 5.967  | 1.00 | 0.00 | 3A7 |
| ATOM | 505 | CG  | ARG | 105 | 26.214 | -25.018 | 6.037  | 1.00 | 0.00 | 3A7 |
| ATOM | 506 | CD  | ARG | 105 | 25.300 | -24.418 | 7.111  | 1.00 | 0.00 | 3A7 |
| ATOM | 507 | NE  | ARG | 105 | 24.029 | -25.205 | 7.173  | 1.00 | 0.00 | 3A7 |
| ATOM | 508 | CZ  | ARG | 105 | 23.007 | -24.845 | 8.007  | 1.00 | 0.00 | 3A7 |
| ATOM | 509 | NH1 | ARG | 105 | 21.860 | -25.583 | 8.027  | 1.00 | 0.00 | 3A7 |
| ATOM | 510 | NH2 | ARG | 105 | 23.124 | -23.752 | 8.816  | 1.00 | 0.00 | 3A7 |
| ATOM | 511 | C   | ARG | 105 | 29.756 | -23.977 | 4.884  | 1.00 | 0.00 | 3A7 |
| ATOM | 512 | O   | ARG | 105 | 30.703 | -24.170 | 5.645  | 1.00 | 0.00 | 3A7 |
| ATOM | 513 | N   | ARG | 106 | 29.750 | -22.991 | 3.955  | 1.00 | 0.00 | 3A7 |
| ATOM | 514 | CA  | ARG | 106 | 30.909 | -22.177 | 3.639  | 1.00 | 0.00 | 3A7 |
| ATOM | 515 | CB  | ARG | 106 | 30.852 | -21.586 | 2.205  | 1.00 | 0.00 | 3A7 |
| ATOM | 516 | CG  | ARG | 106 | 30.675 | -22.664 | 1.121  | 1.00 | 0.00 | 3A7 |
| ATOM | 517 | CD  | ARG | 106 | 30.504 | -22.088 | -0.292 | 1.00 | 0.00 | 3A7 |
| ATOM | 518 | NE  | ARG | 106 | 31.739 | -21.318 | -0.652 | 1.00 | 0.00 | 3A7 |
| ATOM | 519 | CZ  | ARG | 106 | 31.841 | -20.619 | -1.824 | 1.00 | 0.00 | 3A7 |
| ATOM | 520 | NH1 | ARG | 106 | 32.985 | -19.927 | -2.100 | 1.00 | 0.00 | 3A7 |
| ATOM | 521 | NH2 | ARG | 106 | 30.809 | -20.607 | -2.718 | 1.00 | 0.00 | 3A7 |
| ATOM | 522 | C   | ARG | 106 | 31.190 | -21.087 | 4.647  | 1.00 | 0.00 | 3A7 |
| ATOM | 523 | O   | ARG | 106 | 32.357 | -20.971 | 5.015  | 1.00 | 0.00 | 3A7 |
| ATOM | 524 | N   | PRO | 107 | 30.250 | -20.287 | 5.178  | 1.00 | 0.00 | 3A7 |
| ATOM | 525 | CA  | PRO | 107 | 30.565 | -19.212 | 6.105  | 1.00 | 0.00 | 3A7 |
| ATOM | 526 | CD  | PRO | 107 | 28.890 | -20.159 | 4.663  | 1.00 | 0.00 | 3A7 |
| ATOM | 527 | CB  | PRO | 107 | 29.245 | -18.456 | 6.287  | 1.00 | 0.00 | 3A7 |
| ATOM | 528 | CG  | PRO | 107 | 28.480 | -18.724 | 4.991  | 1.00 | 0.00 | 3A7 |
| ATOM | 529 | C   | PRO | 107 | 31.061 | -19.732 | 7.435  | 1.00 | 0.00 | 3A7 |
| ATOM | 530 | O   | PRO | 107 | 31.834 | -19.045 | 8.098  | 1.00 | 0.00 | 3A7 |
| ATOM | 531 | N   | PHE | 108 | 30.645 | -20.949 | 7.846  | 1.00 | 0.00 | 3A7 |
| ATOM | 532 | CA  | PHE | 108 | 30.989 | -21.534 | 9.116  | 1.00 | 0.00 | 3A7 |

|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 533 | CB  | PHE | 108 | 29.984 | -22.623 | 9.543  | 1.00 | 0.00 | 3A7 |
| ATOM | 534 | CG  | PHE | 108 | 28.575 | -22.099 | 9.639  | 1.00 | 0.00 | 3A7 |
| ATOM | 535 | CD1 | PHE | 108 | 27.823 | -21.852 | 8.488  | 1.00 | 0.00 | 3A7 |
| ATOM | 536 | CD2 | PHE | 108 | 27.969 | -21.924 | 10.885 | 1.00 | 0.00 | 3A7 |
| ATOM | 537 | CE1 | PHE | 108 | 26.496 | -21.446 | 8.575  | 1.00 | 0.00 | 3A7 |
| ATOM | 538 | CE2 | PHE | 108 | 26.638 | -21.528 | 10.976 | 1.00 | 0.00 | 3A7 |
| ATOM | 539 | CZ  | PHE | 108 | 25.898 | -21.298 | 9.821  | 1.00 | 0.00 | 3A7 |
| ATOM | 540 | C   | PHE | 108 | 32.360 | -22.153 | 9.070  | 1.00 | 0.00 | 3A7 |
| ATOM | 541 | O   | PHE | 108 | 33.016 | -22.269 | 10.095 | 1.00 | 0.00 | 3A7 |
| ATOM | 542 | N   | GLY | 109 | 32.846 | -22.555 | 7.875  | 1.00 | 0.00 | 3A7 |
| ATOM | 543 | CA  | GLY | 109 | 34.159 | -23.135 | 7.691  | 1.00 | 0.00 | 3A7 |
| ATOM | 544 | C   | GLY | 109 | 35.333 | -22.254 | 8.056  | 1.00 | 0.00 | 3A7 |
| ATOM | 545 | O   | GLY | 109 | 36.321 | -22.774 | 8.561  | 1.00 | 0.00 | 3A7 |
| ATOM | 546 | N   | PRO | 110 | 35.267 | -20.938 | 7.853  | 1.00 | 0.00 | 3A7 |
| ATOM | 547 | CA  | PRO | 110 | 36.311 | -20.023 | 8.270  | 1.00 | 0.00 | 3A7 |
| ATOM | 548 | CD  | PRO | 110 | 34.680 | -20.430 | 6.620  | 1.00 | 0.00 | 3A7 |
| ATOM | 549 | CB  | PRO | 110 | 35.805 | -18.682 | 7.743  | 1.00 | 0.00 | 3A7 |
| ATOM | 550 | CG  | PRO | 110 | 35.292 | -19.054 | 6.361  | 1.00 | 0.00 | 3A7 |
| ATOM | 551 | C   | PRO | 110 | 36.590 | -19.895 | 9.765  | 1.00 | 0.00 | 3A7 |
| ATOM | 552 | O   | PRO | 110 | 37.717 | -19.525 | 10.094 | 1.00 | 0.00 | 3A7 |
| ATOM | 553 | N   | VAL | 111 | 35.620 | -20.153 | 10.690 | 1.00 | 0.00 | 3A7 |
| ATOM | 554 | CA  | VAL | 111 | 35.799 | -19.847 | 12.107 | 1.00 | 0.00 | 3A7 |
| ATOM | 555 | CB  | VAL | 111 | 34.495 | -19.678 | 12.890 | 1.00 | 0.00 | 3A7 |
| ATOM | 556 | CG1 | VAL | 111 | 33.623 | -18.645 | 12.147 | 1.00 | 0.00 | 3A7 |
| ATOM | 557 | CG2 | VAL | 111 | 33.745 | -21.007 | 13.118 | 1.00 | 0.00 | 3A7 |
| ATOM | 558 | C   | VAL | 111 | 36.707 | -20.855 | 12.787 | 1.00 | 0.00 | 3A7 |
| ATOM | 559 | O   | VAL | 111 | 36.539 | -22.067 | 12.658 | 1.00 | 0.00 | 3A7 |
| ATOM | 560 | N   | GLY | 112 | 37.725 | -20.325 | 13.502 | 1.00 | 0.00 | 3A7 |
| ATOM | 561 | CA  | GLY | 112 | 38.761 | -21.102 | 14.130 | 1.00 | 0.00 | 3A7 |
| ATOM | 562 | C   | GLY | 112 | 40.044 | -20.384 | 13.863 | 1.00 | 0.00 | 3A7 |
| ATOM | 563 | O   | GLY | 112 | 40.101 | -19.155 | 13.891 | 1.00 | 0.00 | 3A7 |
| ATOM | 564 | N   | PHE | 113 | 41.113 | -21.162 | 13.582 | 1.00 | 0.00 | 3A7 |
| ATOM | 565 | CA  | PHE | 113 | 42.395 | -20.640 | 13.182 | 1.00 | 0.00 | 3A7 |
| ATOM | 566 | CB  | PHE | 113 | 43.376 | -20.476 | 14.380 | 1.00 | 0.00 | 3A7 |
| ATOM | 567 | CG  | PHE | 113 | 44.692 | -19.854 | 13.980 | 1.00 | 0.00 | 3A7 |
| ATOM | 568 | CD1 | PHE | 113 | 45.891 | -20.468 | 14.346 | 1.00 | 0.00 | 3A7 |
| ATOM | 569 | CD2 | PHE | 113 | 44.738 | -18.671 | 13.239 | 1.00 | 0.00 | 3A7 |
| ATOM | 570 | CE1 | PHE | 113 | 47.113 | -19.918 | 13.971 | 1.00 | 0.00 | 3A7 |
| ATOM | 571 | CE2 | PHE | 113 | 45.959 | -18.120 | 12.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 572 | CZ  | PHE | 113 | 47.148 | -18.744 | 13.226 | 1.00 | 0.00 | 3A7 |
| ATOM | 573 | C   | PHE | 113 | 42.890 | -21.648 | 12.181 | 1.00 | 0.00 | 3A7 |
| ATOM | 574 | O   | PHE | 113 | 43.853 | -22.372 | 12.431 | 1.00 | 0.00 | 3A7 |
| ATOM | 575 | N   | MET | 114 | 42.193 | -21.708 | 11.011 | 1.00 | 0.00 | 3A7 |
| ATOM | 576 | CA  | MET | 114 | 42.417 | -22.600 | 9.882  | 1.00 | 0.00 | 3A7 |
| ATOM | 577 | CB  | MET | 114 | 43.873 | -22.624 | 9.331  | 1.00 | 0.00 | 3A7 |
| ATOM | 578 | CG  | MET | 114 | 44.322 | -21.313 | 8.647  | 1.00 | 0.00 | 3A7 |
| ATOM | 579 | SD  | MET | 114 | 44.745 | -19.936 | 9.761  | 1.00 | 0.00 | 3A7 |
| ATOM | 580 | CE  | MET | 114 | 45.205 | -18.779 | 8.440  | 1.00 | 0.00 | 3A7 |
| ATOM | 581 | C   | MET | 114 | 41.966 | -24.012 | 10.217 | 1.00 | 0.00 | 3A7 |
| ATOM | 582 | O   | MET | 114 | 41.563 | -24.294 | 11.346 | 1.00 | 0.00 | 3A7 |
| ATOM | 583 | N   | LYS | 115 | 42.028 | -24.924 | 9.208  | 1.00 | 0.00 | 3A7 |
| ATOM | 584 | CA  | LYS | 115 | 41.701 | -26.343 | 9.268  | 1.00 | 0.00 | 3A7 |
| ATOM | 585 | CB  | LYS | 115 | 42.359 | -27.158 | 10.423 | 1.00 | 0.00 | 3A7 |
| ATOM | 586 | CG  | LYS | 115 | 43.868 | -27.432 | 10.251 | 1.00 | 0.00 | 3A7 |
| ATOM | 587 | CD  | LYS | 115 | 44.814 | -26.252 | 10.533 | 1.00 | 0.00 | 3A7 |
| ATOM | 588 | CE  | LYS | 115 | 44.796 | -25.758 | 11.988 | 1.00 | 0.00 | 3A7 |
| ATOM | 589 | NZ  | LYS | 115 | 45.206 | -26.832 | 12.922 | 1.00 | 0.00 | 3A7 |
| ATOM | 590 | C   | LYS | 115 | 40.202 | -26.569 | 9.300  | 1.00 | 0.00 | 3A7 |
| ATOM | 591 | O   | LYS | 115 | 39.622 | -26.979 | 8.297  | 1.00 | 0.00 | 3A7 |
| ATOM | 592 | N   | ASN | 116 | 39.579 | -26.341 | 10.491 | 1.00 | 0.00 | 3A7 |
| ATOM | 593 | CA  | ASN | 116 | 38.192 | -26.560 | 10.889 | 1.00 | 0.00 | 3A7 |
| ATOM | 594 | CB  | ASN | 116 | 37.101 | -25.724 | 10.133 | 1.00 | 0.00 | 3A7 |
| ATOM | 595 | CG  | ASN | 116 | 36.831 | -26.079 | 8.657  | 1.00 | 0.00 | 3A7 |
| ATOM | 596 | OD1 | ASN | 116 | 37.384 | -25.453 | 7.745  | 1.00 | 0.00 | 3A7 |
| ATOM | 597 | ND2 | ASN | 116 | 35.919 | -27.074 | 8.437  | 1.00 | 0.00 | 3A7 |
| ATOM | 598 | C   | ASN | 116 | 37.862 | -28.039 | 10.949 | 1.00 | 0.00 | 3A7 |
| ATOM | 599 | O   | ASN | 116 | 38.029 | -28.777 | 9.979  | 1.00 | 0.00 | 3A7 |
| ATOM | 600 | N   | ALA | 117 | 37.387 | -28.501 | 12.134 | 1.00 | 0.00 | 3A7 |
| ATOM | 601 | CA  | ALA | 117 | 37.152 | -29.900 | 12.415 | 1.00 | 0.00 | 3A7 |
| ATOM | 602 | CB  | ALA | 117 | 37.393 | -30.247 | 13.899 | 1.00 | 0.00 | 3A7 |
| ATOM | 603 | C   | ALA | 117 | 35.750 | -30.294 | 12.024 | 1.00 | 0.00 | 3A7 |
| ATOM | 604 | O   | ALA | 117 | 35.542 | -30.857 | 10.951 | 1.00 | 0.00 | 3A7 |

|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 605 | N   | ILE | 118 | 34.758 | -30.027 | 12.909 | 1.00 | 0.00 | 3A7 |
| ATOM | 606 | CA  | ILE | 118 | 33.403 | -30.498 | 12.732 | 1.00 | 0.00 | 3A7 |
| ATOM | 607 | CB  | ILE | 118 | 33.060 | -31.666 | 13.661 | 1.00 | 0.00 | 3A7 |
| ATOM | 608 | CG2 | ILE | 118 | 33.620 | -32.948 | 13.008 | 1.00 | 0.00 | 3A7 |
| ATOM | 609 | CG1 | ILE | 118 | 33.625 | -31.523 | 15.097 | 1.00 | 0.00 | 3A7 |
| ATOM | 610 | CD  | ILE | 118 | 32.902 | -30.511 | 15.983 | 1.00 | 0.00 | 3A7 |
| ATOM | 611 | C   | ILE | 118 | 32.454 | -29.333 | 12.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 612 | O   | ILE | 118 | 31.481 | -29.399 | 13.643 | 1.00 | 0.00 | 3A7 |
| ATOM | 613 | N   | SER | 119 | 32.700 | -28.231 | 12.139 | 1.00 | 0.00 | 3A7 |
| ATOM | 614 | CA  | SER | 119 | 31.852 | -27.054 | 12.114 | 1.00 | 0.00 | 3A7 |
| ATOM | 615 | CB  | SER | 119 | 32.666 | -25.747 | 11.972 | 1.00 | 0.00 | 3A7 |
| ATOM | 616 | OG  | SER | 119 | 33.544 | -25.595 | 13.079 | 1.00 | 0.00 | 3A7 |
| ATOM | 617 | C   | SER | 119 | 30.902 | -27.178 | 10.949 | 1.00 | 0.00 | 3A7 |
| ATOM | 618 | O   | SER | 119 | 31.063 | -26.507 | 9.930  | 1.00 | 0.00 | 3A7 |
| ATOM | 619 | N   | ILE | 120 | 29.898 | -28.096 | 11.093 | 1.00 | 0.00 | 3A7 |
| ATOM | 620 | CA  | ILE | 120 | 28.963 | -28.576 | 10.086 | 1.00 | 0.00 | 3A7 |
| ATOM | 621 | CB  | ILE | 120 | 28.220 | -27.497 | 9.294  | 1.00 | 0.00 | 3A7 |
| ATOM | 622 | CG2 | ILE | 120 | 27.196 | -28.166 | 8.349  | 1.00 | 0.00 | 3A7 |
| ATOM | 623 | CG1 | ILE | 120 | 27.521 | -26.482 | 10.237 | 1.00 | 0.00 | 3A7 |
| ATOM | 624 | CD  | ILE | 120 | 26.467 | -27.096 | 11.166 | 1.00 | 0.00 | 3A7 |
| ATOM | 625 | C   | ILE | 120 | 29.730 | -29.507 | 9.171  | 1.00 | 0.00 | 3A7 |
| ATOM | 626 | O   | ILE | 120 | 30.456 | -29.081 | 8.276  | 1.00 | 0.00 | 3A7 |
| ATOM | 627 | N   | ALA | 121 | 29.621 | -30.825 | 9.421  | 1.00 | 0.00 | 3A7 |
| ATOM | 628 | CA  | ALA | 121 | 30.540 | -31.779 | 8.845  | 1.00 | 0.00 | 3A7 |
| ATOM | 629 | CB  | ALA | 121 | 31.516 | -32.322 | 9.891  | 1.00 | 0.00 | 3A7 |
| ATOM | 630 | C   | ALA | 121 | 29.781 | -32.895 | 8.190  | 1.00 | 0.00 | 3A7 |
| ATOM | 631 | O   | ALA | 121 | 28.574 | -33.051 | 8.369  | 1.00 | 0.00 | 3A7 |
| ATOM | 632 | N   | GLU | 122 | 30.519 | -33.699 | 7.384  | 1.00 | 0.00 | 3A7 |
| ATOM | 633 | CA  | GLU | 122 | 30.006 | -34.785 | 6.580  | 1.00 | 0.00 | 3A7 |
| ATOM | 634 | CB  | GLU | 122 | 30.832 | -34.988 | 5.292  | 1.00 | 0.00 | 3A7 |
| ATOM | 635 | CG  | GLU | 122 | 31.075 | -33.676 | 4.532  | 1.00 | 0.00 | 3A7 |
| ATOM | 636 | CD  | GLU | 122 | 31.734 | -33.979 | 3.190  | 1.00 | 0.00 | 3A7 |
| ATOM | 637 | OE1 | GLU | 122 | 31.094 | -34.679 | 2.360  | 1.00 | 0.00 | 3A7 |
| ATOM | 638 | OE2 | GLU | 122 | 32.884 | -33.510 | 2.975  | 1.00 | 0.00 | 3A7 |
| ATOM | 639 | C   | GLU | 122 | 30.077 | -36.057 | 7.368  | 1.00 | 0.00 | 3A7 |
| ATOM | 640 | O   | GLU | 122 | 30.753 | -36.091 | 8.393  | 1.00 | 0.00 | 3A7 |
| ATOM | 641 | N   | ASP | 123 | 29.389 | -37.130 | 6.889  | 1.00 | 0.00 | 3A7 |
| ATOM | 642 | CA  | ASP | 123 | 29.236 | -38.402 | 7.576  | 1.00 | 0.00 | 3A7 |
| ATOM | 643 | CB  | ASP | 123 | 27.977 | -39.195 | 7.107  | 1.00 | 0.00 | 3A7 |
| ATOM | 644 | CG  | ASP | 123 | 28.012 | -39.602 | 5.628  | 1.00 | 0.00 | 3A7 |
| ATOM | 645 | OD1 | ASP | 123 | 28.196 | -38.707 | 4.763  | 1.00 | 0.00 | 3A7 |
| ATOM | 646 | OD2 | ASP | 123 | 27.861 | -40.822 | 5.354  | 1.00 | 0.00 | 3A7 |
| ATOM | 647 | C   | ASP | 123 | 30.485 | -39.259 | 7.471  | 1.00 | 0.00 | 3A7 |
| ATOM | 648 | O   | ASP | 123 | 30.724 | -39.955 | 6.485  | 1.00 | 0.00 | 3A7 |
| ATOM | 649 | N   | GLU | 124 | 31.302 | -39.189 | 8.540  | 1.00 | 0.00 | 3A7 |
| ATOM | 650 | CA  | GLU | 124 | 32.560 | -39.870 | 8.683  | 1.00 | 0.00 | 3A7 |
| ATOM | 651 | CB  | GLU | 124 | 33.626 | -39.519 | 7.609  | 1.00 | 0.00 | 3A7 |
| ATOM | 652 | CG  | GLU | 124 | 34.965 | -40.257 | 7.793  | 1.00 | 0.00 | 3A7 |
| ATOM | 653 | CD  | GLU | 124 | 35.918 | -39.851 | 6.672  | 1.00 | 0.00 | 3A7 |
| ATOM | 654 | OE1 | GLU | 124 | 36.993 | -39.275 | 6.989  | 1.00 | 0.00 | 3A7 |
| ATOM | 655 | OE2 | GLU | 124 | 35.585 | -40.115 | 5.486  | 1.00 | 0.00 | 3A7 |
| ATOM | 656 | C   | GLU | 124 | 33.018 | -39.381 | 10.020 | 1.00 | 0.00 | 3A7 |
| ATOM | 657 | O   | GLU | 124 | 33.474 | -40.149 | 10.866 | 1.00 | 0.00 | 3A7 |
| ATOM | 658 | N   | GLU | 125 | 32.873 | -38.047 | 10.219 | 1.00 | 0.00 | 3A7 |
| ATOM | 659 | CA  | GLU | 125 | 33.141 | -37.358 | 11.455 | 1.00 | 0.00 | 3A7 |
| ATOM | 660 | CB  | GLU | 125 | 33.984 | -36.078 | 11.267 | 1.00 | 0.00 | 3A7 |
| ATOM | 661 | CG  | GLU | 125 | 35.301 | -36.303 | 10.505 | 1.00 | 0.00 | 3A7 |
| ATOM | 662 | CD  | GLU | 125 | 36.159 | -37.314 | 11.254 | 1.00 | 0.00 | 3A7 |
| ATOM | 663 | OE1 | GLU | 125 | 36.439 | -38.392 | 10.667 | 1.00 | 0.00 | 3A7 |
| ATOM | 664 | OE2 | GLU | 125 | 36.546 | -37.024 | 12.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 665 | C   | GLU | 125 | 31.844 | -36.969 | 12.096 | 1.00 | 0.00 | 3A7 |
| ATOM | 666 | O   | GLU | 125 | 31.785 | -36.775 | 13.306 | 1.00 | 0.00 | 3A7 |
| ATOM | 667 | N   | TRP | 126 | 30.739 | -36.843 | 11.315 | 1.00 | 0.00 | 3A7 |
| ATOM | 668 | CA  | TRP | 126 | 29.448 | -36.458 | 11.855 | 1.00 | 0.00 | 3A7 |
| ATOM | 669 | CB  | TRP | 126 | 28.460 | -36.001 | 10.762 | 1.00 | 0.00 | 3A7 |
| ATOM | 670 | CG  | TRP | 126 | 27.427 | -34.955 | 11.159 | 1.00 | 0.00 | 3A7 |
| ATOM | 671 | CD2 | TRP | 126 | 27.726 | -33.684 | 11.776 | 1.00 | 0.00 | 3A7 |
| ATOM | 672 | CD1 | TRP | 126 | 26.092 | -34.933 | 10.869 | 1.00 | 0.00 | 3A7 |
| ATOM | 673 | NE1 | TRP | 126 | 25.536 | -33.741 | 11.271 | 1.00 | 0.00 | 3A7 |
| ATOM | 674 | CE2 | TRP | 126 | 26.527 | -32.954 | 11.818 | 1.00 | 0.00 | 3A7 |
| ATOM | 675 | CE3 | TRP | 126 | 28.905 | -33.139 | 12.252 | 1.00 | 0.00 | 3A7 |
| ATOM | 676 | CZ2 | TRP | 126 | 26.494 | -31.670 | 12.329 | 1.00 | 0.00 | 3A7 |

|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 677 | CZ3 | TRP | 126 | 28.868 | -31.850 | 12.774 | 1.00 | 0.00 | 3A7 |
| ATOM | 678 | CH2 | TRP | 126 | 27.680 | -31.123 | 12.810 | 1.00 | 0.00 | 3A7 |
| ATOM | 679 | C   | TRP | 126 | 28.874 | -37.602 | 12.636 | 1.00 | 0.00 | 3A7 |
| ATOM | 680 | O   | TRP | 126 | 28.393 | -37.423 | 13.750 | 1.00 | 0.00 | 3A7 |
| ATOM | 681 | N   | LYS | 127 | 28.962 | -38.842 | 12.090 | 1.00 | 0.00 | 3A7 |
| ATOM | 682 | CA  | LYS | 127 | 28.511 | -40.060 | 12.743 | 1.00 | 0.00 | 3A7 |
| ATOM | 683 | CB  | LYS | 127 | 28.749 | -41.279 | 11.833 | 1.00 | 0.00 | 3A7 |
| ATOM | 684 | CG  | LYS | 127 | 28.086 | -42.581 | 12.315 | 1.00 | 0.00 | 3A7 |
| ATOM | 685 | CD  | LYS | 127 | 28.264 | -43.736 | 11.316 | 1.00 | 0.00 | 3A7 |
| ATOM | 686 | CE  | LYS | 127 | 27.607 | -45.046 | 11.770 | 1.00 | 0.00 | 3A7 |
| ATOM | 687 | NZ  | LYS | 127 | 26.139 | -44.893 | 11.883 | 1.00 | 0.00 | 3A7 |
| ATOM | 688 | C   | LYS | 127 | 29.196 | -40.320 | 14.072 | 1.00 | 0.00 | 3A7 |
| ATOM | 689 | O   | LYS | 127 | 28.561 | -40.651 | 15.070 | 1.00 | 0.00 | 3A7 |
| ATOM | 690 | N   | ARG | 128 | 30.530 | -40.112 | 14.123 | 1.00 | 0.00 | 3A7 |
| ATOM | 691 | CA  | ARG | 128 | 31.301 | -40.271 | 15.331 | 1.00 | 0.00 | 3A7 |
| ATOM | 692 | CB  | ARG | 128 | 32.812 | -40.274 | 15.061 | 1.00 | 0.00 | 3A7 |
| ATOM | 693 | CG  | ARG | 128 | 33.252 | -41.515 | 14.267 | 1.00 | 0.00 | 3A7 |
| ATOM | 694 | CD  | ARG | 128 | 34.765 | -41.777 | 14.317 | 1.00 | 0.00 | 3A7 |
| ATOM | 695 | NE  | ARG | 128 | 35.198 | -41.942 | 15.749 | 1.00 | 0.00 | 3A7 |
| ATOM | 696 | CZ  | ARG | 128 | 34.997 | -43.090 | 16.469 | 1.00 | 0.00 | 3A7 |
| ATOM | 697 | NH1 | ARG | 128 | 35.389 | -43.140 | 17.776 | 1.00 | 0.00 | 3A7 |
| ATOM | 698 | NH2 | ARG | 128 | 34.422 | -44.186 | 15.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 699 | C   | ARG | 128 | 30.991 | -39.217 | 16.367 | 1.00 | 0.00 | 3A7 |
| ATOM | 700 | O   | ARG | 128 | 30.847 | -39.549 | 17.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 701 | N   | ILE | 129 | 30.823 | -37.931 | 15.976 | 1.00 | 0.00 | 3A7 |
| ATOM | 702 | CA  | ILE | 129 | 30.486 | -36.852 | 16.897 | 1.00 | 0.00 | 3A7 |
| ATOM | 703 | CB  | ILE | 129 | 30.651 | -35.498 | 16.229 | 1.00 | 0.00 | 3A7 |
| ATOM | 704 | CG2 | ILE | 129 | 29.684 | -34.398 | 16.740 | 1.00 | 0.00 | 3A7 |
| ATOM | 705 | CG1 | ILE | 129 | 32.104 | -34.975 | 16.405 | 1.00 | 0.00 | 3A7 |
| ATOM | 706 | CD  | ILE | 129 | 33.250 | -35.944 | 16.093 | 1.00 | 0.00 | 3A7 |
| ATOM | 707 | C   | ILE | 129 | 29.095 | -37.028 | 17.444 | 1.00 | 0.00 | 3A7 |
| ATOM | 708 | O   | ILE | 129 | 28.882 | -36.896 | 18.640 | 1.00 | 0.00 | 3A7 |
| ATOM | 709 | N   | ARG | 130 | 28.114 | -37.398 | 16.595 | 1.00 | 0.00 | 3A7 |
| ATOM | 710 | CA  | ARG | 130 | 26.759 | -37.661 | 17.021 | 1.00 | 0.00 | 3A7 |
| ATOM | 711 | CB  | ARG | 130 | 25.849 | -37.943 | 15.811 | 1.00 | 0.00 | 3A7 |
| ATOM | 712 | CG  | ARG | 130 | 25.540 | -36.681 | 14.987 | 1.00 | 0.00 | 3A7 |
| ATOM | 713 | CD  | ARG | 130 | 24.607 | -36.942 | 13.796 | 1.00 | 0.00 | 3A7 |
| ATOM | 714 | NE  | ARG | 130 | 25.280 | -37.896 | 12.857 | 1.00 | 0.00 | 3A7 |
| ATOM | 715 | CZ  | ARG | 130 | 24.691 | -38.311 | 11.694 | 1.00 | 0.00 | 3A7 |
| ATOM | 716 | NH1 | ARG | 130 | 25.358 | -39.169 | 10.868 | 1.00 | 0.00 | 3A7 |
| ATOM | 717 | NH2 | ARG | 130 | 23.446 | -37.869 | 11.351 | 1.00 | 0.00 | 3A7 |
| ATOM | 718 | C   | ARG | 130 | 26.695 | -38.843 | 17.970 | 1.00 | 0.00 | 3A7 |
| ATOM | 719 | O   | ARG | 130 | 26.037 | -38.756 | 18.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 720 | N   | SER | 131 | 27.443 | -39.943 | 17.701 | 1.00 | 0.00 | 3A7 |
| ATOM | 721 | CA  | SER | 131 | 27.492 | -41.105 | 18.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 722 | CB  | SER | 131 | 28.322 | -42.268 | 17.985 | 1.00 | 0.00 | 3A7 |
| ATOM | 723 | OG  | SER | 131 | 29.697 | -41.986 | 17.760 | 1.00 | 0.00 | 3A7 |
| ATOM | 724 | C   | SER | 131 | 28.053 | -40.816 | 19.936 | 1.00 | 0.00 | 3A7 |
| ATOM | 725 | O   | SER | 131 | 27.615 | -41.352 | 20.947 | 1.00 | 0.00 | 3A7 |
| ATOM | 726 | N   | LEU | 132 | 29.066 | -39.936 | 19.998 | 1.00 | 0.00 | 3A7 |
| ATOM | 727 | CA  | LEU | 132 | 29.705 | -39.583 | 21.240 | 1.00 | 0.00 | 3A7 |
| ATOM | 728 | CB  | LEU | 132 | 31.017 | -38.838 | 20.968 | 1.00 | 0.00 | 3A7 |
| ATOM | 729 | CG  | LEU | 132 | 32.105 | -39.732 | 20.333 | 1.00 | 0.00 | 3A7 |
| ATOM | 730 | CD1 | LEU | 132 | 33.135 | -38.875 | 19.583 | 1.00 | 0.00 | 3A7 |
| ATOM | 731 | CD2 | LEU | 132 | 32.782 | -40.648 | 21.366 | 1.00 | 0.00 | 3A7 |
| ATOM | 732 | C   | LEU | 132 | 28.808 | -38.721 | 22.089 | 1.00 | 0.00 | 3A7 |
| ATOM | 733 | O   | LEU | 132 | 28.688 | -38.937 | 23.289 | 1.00 | 0.00 | 3A7 |
| ATOM | 734 | N   | LEU | 133 | 28.116 | -37.745 | 21.460 | 1.00 | 0.00 | 3A7 |
| ATOM | 735 | CA  | LEU | 133 | 27.269 | -36.794 | 22.145 | 1.00 | 0.00 | 3A7 |
| ATOM | 736 | CB  | LEU | 133 | 26.997 | -35.547 | 21.272 | 1.00 | 0.00 | 3A7 |
| ATOM | 737 | CG  | LEU | 133 | 28.266 | -34.787 | 20.869 | 1.00 | 0.00 | 3A7 |
| ATOM | 738 | CD1 | LEU | 133 | 27.918 | -33.493 | 20.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 739 | CD2 | LEU | 133 | 29.211 | -34.589 | 22.052 | 1.00 | 0.00 | 3A7 |
| ATOM | 740 | C   | LEU | 133 | 25.928 | -37.334 | 22.547 | 1.00 | 0.00 | 3A7 |
| ATOM | 741 | O   | LEU | 133 | 25.403 | -36.955 | 23.590 | 1.00 | 0.00 | 3A7 |
| ATOM | 742 | N   | SER | 134 | 25.333 | -38.237 | 21.738 | 1.00 | 0.00 | 3A7 |
| ATOM | 743 | CA  | SER | 134 | 24.003 | -38.748 | 21.970 | 1.00 | 0.00 | 3A7 |
| ATOM | 744 | CB  | SER | 134 | 23.511 | -39.662 | 20.844 | 1.00 | 0.00 | 3A7 |
| ATOM | 745 | OG  | SER | 134 | 24.394 | -40.706 | 20.461 | 1.00 | 0.00 | 3A7 |
| ATOM | 746 | C   | SER | 134 | 23.800 | -39.430 | 23.296 | 1.00 | 0.00 | 3A7 |
| ATOM | 747 | O   | SER | 134 | 22.725 | -39.226 | 23.854 | 1.00 | 0.00 | 3A7 |
| ATOM | 748 | N   | PRO | 135 | 24.715 | -40.198 | 23.891 | 1.00 | 0.00 | 3A7 |

|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 749 | CA  | PRO | 135 | 24.491 | -40.773 | 25.190 | 1.00 | 0.00 | 3A7 |
| ATOM | 750 | CD  | PRO | 135 | 25.854 | -40.834 | 23.260 | 1.00 | 0.00 | 3A7 |
| ATOM | 751 | CB  | PRO | 135 | 25.551 | -41.871 | 25.355 | 1.00 | 0.00 | 3A7 |
| ATOM | 752 | CG  | PRO | 135 | 25.961 | -42.203 | 23.924 | 1.00 | 0.00 | 3A7 |
| ATOM | 753 | C   | PRO | 135 | 24.618 | -39.783 | 26.310 | 1.00 | 0.00 | 3A7 |
| ATOM | 754 | O   | PRO | 135 | 23.867 | -39.912 | 27.273 | 1.00 | 0.00 | 3A7 |
| ATOM | 755 | N   | THR | 136 | 25.553 | -38.805 | 26.231 | 1.00 | 0.00 | 3A7 |
| ATOM | 756 | CA  | THR | 136 | 25.770 | -37.840 | 27.291 | 1.00 | 0.00 | 3A7 |
| ATOM | 757 | CB  | THR | 136 | 27.148 | -37.210 | 27.207 | 1.00 | 0.00 | 3A7 |
| ATOM | 758 | OG1 | THR | 136 | 27.386 | -36.654 | 25.918 | 1.00 | 0.00 | 3A7 |
| ATOM | 759 | CG2 | THR | 136 | 28.182 | -38.319 | 27.492 | 1.00 | 0.00 | 3A7 |
| ATOM | 760 | C   | THR | 136 | 24.693 | -36.769 | 27.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 761 | O   | THR | 136 | 24.369 | -36.212 | 28.360 | 1.00 | 0.00 | 3A7 |
| ATOM | 762 | N   | PHE | 137 | 24.066 | -36.471 | 26.165 | 1.00 | 0.00 | 3A7 |
| ATOM | 763 | CA  | PHE | 137 | 23.044 | -35.454 | 26.069 | 1.00 | 0.00 | 3A7 |
| ATOM | 764 | CB  | PHE | 137 | 23.219 | -34.665 | 24.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 765 | CG  | PHE | 137 | 24.305 | -33.645 | 25.018 | 1.00 | 0.00 | 3A7 |
| ATOM | 766 | CD1 | PHE | 137 | 25.578 | -33.792 | 24.468 | 1.00 | 0.00 | 3A7 |
| ATOM | 767 | CD2 | PHE | 137 | 24.057 | -32.535 | 25.831 | 1.00 | 0.00 | 3A7 |
| ATOM | 768 | CE1 | PHE | 137 | 26.580 | -32.863 | 24.725 | 1.00 | 0.00 | 3A7 |
| ATOM | 769 | CE2 | PHE | 137 | 25.050 | -31.590 | 26.070 | 1.00 | 0.00 | 3A7 |
| ATOM | 770 | CZ  | PHE | 137 | 26.316 | -31.757 | 25.524 | 1.00 | 0.00 | 3A7 |
| ATOM | 771 | C   | PHE | 137 | 21.711 | -36.153 | 26.100 | 1.00 | 0.00 | 3A7 |
| ATOM | 772 | O   | PHE | 137 | 20.779 | -35.799 | 25.406 | 1.00 | 0.00 | 3A7 |
| ATOM | 773 | N   | THR | 138 | 21.542 | -37.179 | 26.952 | 1.00 | 0.00 | 3A7 |
| ATOM | 774 | CA  | THR | 138 | 20.246 | -37.782 | 27.179 | 1.00 | 0.00 | 3A7 |
| ATOM | 775 | CB  | THR | 138 | 20.313 | -39.259 | 27.505 | 1.00 | 0.00 | 3A7 |
| ATOM | 776 | OG1 | THR | 138 | 21.270 | -39.549 | 28.518 | 1.00 | 0.00 | 3A7 |
| ATOM | 777 | CG2 | THR | 138 | 20.673 | -40.035 | 26.226 | 1.00 | 0.00 | 3A7 |
| ATOM | 778 | C   | THR | 138 | 19.588 | -37.063 | 28.326 | 1.00 | 0.00 | 3A7 |
| ATOM | 779 | O   | THR | 138 | 20.234 | -36.412 | 29.149 | 1.00 | 0.00 | 3A7 |
| ATOM | 780 | N   | SER | 139 | 18.250 | -37.211 | 28.416 | 1.00 | 0.00 | 3A7 |
| ATOM | 781 | CA  | SER | 139 | 17.433 | -36.585 | 29.427 | 1.00 | 0.00 | 3A7 |
| ATOM | 782 | CB  | SER | 139 | 15.917 | -36.809 | 29.183 | 1.00 | 0.00 | 3A7 |
| ATOM | 783 | OG  | SER | 139 | 15.590 | -38.188 | 29.037 | 1.00 | 0.00 | 3A7 |
| ATOM | 784 | C   | SER | 139 | 17.797 | -37.053 | 30.810 | 1.00 | 0.00 | 3A7 |
| ATOM | 785 | O   | SER | 139 | 17.738 | -36.290 | 31.765 | 1.00 | 0.00 | 3A7 |
| ATOM | 786 | N   | GLY | 140 | 18.263 | -38.318 | 30.922 | 1.00 | 0.00 | 3A7 |
| ATOM | 787 | CA  | GLY | 140 | 18.713 | -38.898 | 32.158 | 1.00 | 0.00 | 3A7 |
| ATOM | 788 | C   | GLY | 140 | 20.032 | -38.362 | 32.618 | 1.00 | 0.00 | 3A7 |
| ATOM | 789 | O   | GLY | 140 | 20.273 | -38.260 | 33.820 | 1.00 | 0.00 | 3A7 |
| ATOM | 790 | N   | LYS | 141 | 20.933 | -38.021 | 31.673 | 1.00 | 0.00 | 3A7 |
| ATOM | 791 | CA  | LYS | 141 | 22.309 | -37.803 | 32.064 | 1.00 | 0.00 | 3A7 |
| ATOM | 792 | CB  | LYS | 141 | 23.285 | -38.611 | 31.169 | 1.00 | 0.00 | 3A7 |
| ATOM | 793 | CG  | LYS | 141 | 23.070 | -40.129 | 31.293 | 1.00 | 0.00 | 3A7 |
| ATOM | 794 | CD  | LYS | 141 | 24.150 | -40.944 | 30.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 795 | CE  | LYS | 141 | 23.916 | -42.456 | 30.655 | 1.00 | 0.00 | 3A7 |
| ATOM | 796 | NZ  | LYS | 141 | 24.978 | -43.189 | 29.928 | 1.00 | 0.00 | 3A7 |
| ATOM | 797 | C   | LYS | 141 | 22.832 | -36.386 | 32.232 | 1.00 | 0.00 | 3A7 |
| ATOM | 798 | O   | LYS | 141 | 22.859 | -35.680 | 33.265 | 1.00 | 0.00 | 3A7 |
| ATOM | 799 | N   | LEU | 142 | 23.635 | -36.031 | 31.185 | 1.00 | 0.00 | 3A7 |
| ATOM | 800 | CA  | LEU | 142 | 24.644 | -34.970 | 31.099 | 1.00 | 0.00 | 3A7 |
| ATOM | 801 | CB  | LEU | 142 | 23.972 | -33.593 | 30.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 802 | CG  | LEU | 142 | 24.455 | -32.799 | 29.656 | 1.00 | 0.00 | 3A7 |
| ATOM | 803 | CD1 | LEU | 142 | 23.560 | -31.564 | 29.439 | 1.00 | 0.00 | 3A7 |
| ATOM | 804 | CD2 | LEU | 142 | 25.943 | -32.407 | 29.718 | 1.00 | 0.00 | 3A7 |
| ATOM | 805 | C   | LEU | 142 | 25.663 | -34.903 | 32.241 | 1.00 | 0.00 | 3A7 |
| ATOM | 806 | O   | LEU | 142 | 26.359 | -33.901 | 32.398 | 1.00 | 0.00 | 3A7 |
| ATOM | 807 | N   | LYS | 143 | 25.729 | -35.975 | 33.085 | 1.00 | 0.00 | 3A7 |
| ATOM | 808 | CA  | LYS | 143 | 26.391 | -36.077 | 34.381 | 1.00 | 0.00 | 3A7 |
| ATOM | 809 | CB  | LYS | 143 | 27.931 | -35.966 | 34.315 | 1.00 | 0.00 | 3A7 |
| ATOM | 810 | CG  | LYS | 143 | 28.567 | -37.003 | 33.373 | 1.00 | 0.00 | 3A7 |
| ATOM | 811 | CD  | LYS | 143 | 28.188 | -38.480 | 33.614 | 1.00 | 0.00 | 3A7 |
| ATOM | 812 | CE  | LYS | 143 | 28.784 | -39.129 | 34.873 | 1.00 | 0.00 | 3A7 |
| ATOM | 813 | NZ  | LYS | 143 | 28.177 | -38.601 | 36.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 814 | C   | LYS | 143 | 25.831 | -35.060 | 35.351 | 1.00 | 0.00 | 3A7 |
| ATOM | 815 | O   | LYS | 143 | 26.561 | -34.248 | 35.919 | 1.00 | 0.00 | 3A7 |
| ATOM | 816 | N   | GLU | 144 | 24.476 | -35.097 | 35.479 | 1.00 | 0.00 | 3A7 |
| ATOM | 817 | CA  | GLU | 144 | 23.593 | -34.122 | 36.090 | 1.00 | 0.00 | 3A7 |
| ATOM | 818 | CB  | GLU | 144 | 24.058 | -33.575 | 37.466 | 1.00 | 0.00 | 3A7 |
| ATOM | 819 | CG  | GLU | 144 | 24.205 | -34.669 | 38.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 820 | CD  | GLU | 144 | 24.730 | -34.037 | 39.820 | 1.00 | 0.00 | 3A7 |



|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 821 | OE1 | GLU | 144 | 25.849 | -34.422 | 40.255 | 1.00 | 0.00 | 3A7 |
| ATOM | 822 | OE2 | GLU | 144 | 24.022 | -33.161 | 40.384 | 1.00 | 0.00 | 3A7 |
| ATOM | 823 | C   | GLU | 144 | 23.380 | -32.972 | 35.123 | 1.00 | 0.00 | 3A7 |
| ATOM | 824 | O   | GLU | 144 | 24.284 | -32.166 | 34.907 | 1.00 | 0.00 | 3A7 |
| ATOM | 825 | N   | MET | 145 | 22.163 | -32.867 | 34.523 | 1.00 | 0.00 | 3A7 |
| ATOM | 826 | CA  | MET | 145 | 21.768 | -31.691 | 33.757 | 1.00 | 0.00 | 3A7 |
| ATOM | 827 | CB  | MET | 145 | 21.203 | -31.937 | 32.347 | 1.00 | 0.00 | 3A7 |
| ATOM | 828 | CG  | MET | 145 | 20.243 | -33.140 | 32.238 | 1.00 | 0.00 | 3A7 |
| ATOM | 829 | SD  | MET | 145 | 19.496 | -33.350 | 30.593 | 1.00 | 0.00 | 3A7 |
| ATOM | 830 | CE  | MET | 145 | 18.314 | -31.978 | 30.743 | 1.00 | 0.00 | 3A7 |
| ATOM | 831 | C   | MET | 145 | 20.736 | -30.926 | 34.510 | 1.00 | 0.00 | 3A7 |
| ATOM | 832 | O   | MET | 145 | 20.810 | -29.704 | 34.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 833 | N   | VAL | 146 | 19.718 | -31.609 | 35.082 | 1.00 | 0.00 | 3A7 |
| ATOM | 834 | CA  | VAL | 146 | 18.618 | -30.943 | 35.756 | 1.00 | 0.00 | 3A7 |
| ATOM | 835 | CB  | VAL | 146 | 17.494 | -31.869 | 36.146 | 1.00 | 0.00 | 3A7 |
| ATOM | 836 | CG1 | VAL | 146 | 16.290 | -30.982 | 36.556 | 1.00 | 0.00 | 3A7 |
| ATOM | 837 | CG2 | VAL | 146 | 17.145 | -32.759 | 34.935 | 1.00 | 0.00 | 3A7 |
| ATOM | 838 | C   | VAL | 146 | 19.066 | -30.148 | 36.957 | 1.00 | 0.00 | 3A7 |
| ATOM | 839 | O   | VAL | 146 | 18.633 | -29.004 | 37.094 | 1.00 | 0.00 | 3A7 |
| ATOM | 840 | N   | PRO | 147 | 19.976 | -30.644 | 37.801 | 1.00 | 0.00 | 3A7 |
| ATOM | 841 | CA  | PRO | 147 | 20.491 | -29.872 | 38.908 | 1.00 | 0.00 | 3A7 |
| ATOM | 842 | CD  | PRO | 147 | 20.305 | -32.060 | 37.960 | 1.00 | 0.00 | 3A7 |
| ATOM | 843 | CB  | PRO | 147 | 21.360 | -30.856 | 39.708 | 1.00 | 0.00 | 3A7 |
| ATOM | 844 | CG  | PRO | 147 | 20.726 | -32.213 | 39.420 | 1.00 | 0.00 | 3A7 |
| ATOM | 845 | C   | PRO | 147 | 21.286 | -28.672 | 38.470 | 1.00 | 0.00 | 3A7 |
| ATOM | 846 | O   | PRO | 147 | 21.286 | -27.680 | 39.190 | 1.00 | 0.00 | 3A7 |
| ATOM | 847 | N   | ILE | 148 | 21.943 | -28.722 | 37.294 | 1.00 | 0.00 | 3A7 |
| ATOM | 848 | CA  | ILE | 148 | 22.723 | -27.631 | 36.762 | 1.00 | 0.00 | 3A7 |
| ATOM | 849 | CB  | ILE | 148 | 23.664 | -28.114 | 35.675 | 1.00 | 0.00 | 3A7 |
| ATOM | 850 | CG2 | ILE | 148 | 24.341 | -26.923 | 34.952 | 1.00 | 0.00 | 3A7 |
| ATOM | 851 | CG1 | ILE | 148 | 24.796 | -29.020 | 36.211 | 1.00 | 0.00 | 3A7 |
| ATOM | 852 | CD  | ILE | 148 | 24.460 | -30.116 | 37.225 | 1.00 | 0.00 | 3A7 |
| ATOM | 853 | C   | ILE | 148 | 21.813 | -26.558 | 36.204 | 1.00 | 0.00 | 3A7 |
| ATOM | 854 | O   | ILE | 148 | 22.073 | -25.361 | 36.322 | 1.00 | 0.00 | 3A7 |
| ATOM | 855 | N   | ILE | 149 | 20.672 | -26.968 | 35.607 | 1.00 | 0.00 | 3A7 |
| ATOM | 856 | CA  | ILE | 149 | 19.682 | -26.045 | 35.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 857 | CB  | ILE | 149 | 18.645 | -26.744 | 34.263 | 1.00 | 0.00 | 3A7 |
| ATOM | 858 | CG2 | ILE | 149 | 17.595 | -25.733 | 33.743 | 1.00 | 0.00 | 3A7 |
| ATOM | 859 | CG1 | ILE | 149 | 19.377 | -27.390 | 33.058 | 1.00 | 0.00 | 3A7 |
| ATOM | 860 | CD  | ILE | 149 | 18.552 | -28.444 | 32.319 | 1.00 | 0.00 | 3A7 |
| ATOM | 861 | C   | ILE | 149 | 19.032 | -25.338 | 36.240 | 1.00 | 0.00 | 3A7 |
| ATOM | 862 | O   | ILE | 149 | 18.779 | -24.137 | 36.179 | 1.00 | 0.00 | 3A7 |
| ATOM | 863 | N   | ALA | 150 | 18.793 | -26.059 | 37.357 | 1.00 | 0.00 | 3A7 |
| ATOM | 864 | CA  | ALA | 150 | 18.229 | -25.493 | 38.558 | 1.00 | 0.00 | 3A7 |
| ATOM | 865 | CB  | ALA | 150 | 17.894 | -26.586 | 39.578 | 1.00 | 0.00 | 3A7 |
| ATOM | 866 | C   | ALA | 150 | 19.160 | -24.490 | 39.195 | 1.00 | 0.00 | 3A7 |
| ATOM | 867 | O   | ALA | 150 | 18.723 | -23.461 | 39.693 | 1.00 | 0.00 | 3A7 |
| ATOM | 868 | N   | GLN | 151 | 20.488 | -24.737 | 39.144 | 1.00 | 0.00 | 3A7 |
| ATOM | 869 | CA  | GLN | 151 | 21.492 | -23.836 | 39.661 | 1.00 | 0.00 | 3A7 |
| ATOM | 870 | CB  | GLN | 151 | 22.910 | -24.428 | 39.555 | 1.00 | 0.00 | 3A7 |
| ATOM | 871 | CG  | GLN | 151 | 23.192 | -25.483 | 40.637 | 1.00 | 0.00 | 3A7 |
| ATOM | 872 | CD  | GLN | 151 | 24.551 | -26.129 | 40.357 | 1.00 | 0.00 | 3A7 |
| ATOM | 873 | OE1 | GLN | 151 | 25.580 | -25.444 | 40.306 | 1.00 | 0.00 | 3A7 |
| ATOM | 874 | NE2 | GLN | 151 | 24.541 | -27.485 | 40.172 | 1.00 | 0.00 | 3A7 |
| ATOM | 875 | C   | GLN | 151 | 21.475 | -22.493 | 38.989 | 1.00 | 0.00 | 3A7 |
| ATOM | 876 | O   | GLN | 151 | 21.418 | -21.447 | 39.634 | 1.00 | 0.00 | 3A7 |
| ATOM | 877 | N   | TYR | 152 | 21.474 | -22.502 | 37.644 | 1.00 | 0.00 | 3A7 |
| ATOM | 878 | CA  | TYR | 152 | 21.438 | -21.288 | 36.872 | 1.00 | 0.00 | 3A7 |
| ATOM | 879 | CB  | TYR | 152 | 21.651 | -21.508 | 35.367 | 1.00 | 0.00 | 3A7 |
| ATOM | 880 | CG  | TYR | 152 | 22.236 | -20.216 | 34.776 | 1.00 | 0.00 | 3A7 |
| ATOM | 881 | CD1 | TYR | 152 | 23.578 | -19.994 | 35.099 | 1.00 | 0.00 | 3A7 |
| ATOM | 882 | CD2 | TYR | 152 | 21.411 | -19.109 | 34.632 | 1.00 | 0.00 | 3A7 |
| ATOM | 883 | CE1 | TYR | 152 | 24.053 | -18.705 | 35.335 | 1.00 | 0.00 | 3A7 |
| ATOM | 884 | CE2 | TYR | 152 | 21.870 | -17.822 | 34.898 | 1.00 | 0.00 | 3A7 |
| ATOM | 885 | CZ  | TYR | 152 | 23.208 | -17.612 | 35.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 886 | OH  | TYR | 152 | 23.690 | -16.302 | 35.411 | 1.00 | 0.00 | 3A7 |
| ATOM | 887 | C   | TYR | 152 | 20.140 | -20.556 | 37.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 888 | O   | TYR | 152 | 20.108 | -19.335 | 37.134 | 1.00 | 0.00 | 3A7 |
| ATOM | 889 | N   | GLY | 153 | 19.025 | -21.301 | 37.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 890 | CA  | GLY | 153 | 17.715 | -20.733 | 37.311 | 1.00 | 0.00 | 3A7 |
| ATOM | 891 | C   | GLY | 153 | 17.596 | -19.972 | 38.591 | 1.00 | 0.00 | 3A7 |
| ATOM | 892 | O   | GLY | 153 | 16.977 | -18.915 | 38.657 | 1.00 | 0.00 | 3A7 |

|      |     |     |     |     |        |         |        |      |      |     |
|------|-----|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 893 | N   | ASP | 154 | 18.270 | -20.457 | 39.650 | 1.00 | 0.00 | 3A7 |
| ATOM | 894 | CA  | ASP | 154 | 18.353 | -19.782 | 40.919 | 1.00 | 0.00 | 3A7 |
| ATOM | 895 | CB  | ASP | 154 | 19.017 | -20.685 | 41.976 | 1.00 | 0.00 | 3A7 |
| ATOM | 896 | CG  | ASP | 154 | 18.142 | -21.901 | 42.299 | 1.00 | 0.00 | 3A7 |
| ATOM | 897 | OD1 | ASP | 154 | 16.975 | -21.960 | 41.830 | 1.00 | 0.00 | 3A7 |
| ATOM | 898 | OD2 | ASP | 154 | 18.643 | -22.790 | 43.039 | 1.00 | 0.00 | 3A7 |
| ATOM | 899 | C   | ASP | 154 | 19.130 | -18.483 | 40.808 | 1.00 | 0.00 | 3A7 |
| ATOM | 900 | O   | ASP | 154 | 18.726 | -17.469 | 41.361 | 1.00 | 0.00 | 3A7 |
| ATOM | 901 | N   | VAL | 155 | 20.243 | -18.474 | 40.041 | 1.00 | 0.00 | 3A7 |
| ATOM | 902 | CA  | VAL | 155 | 21.039 | -17.293 | 39.761 | 1.00 | 0.00 | 3A7 |
| ATOM | 903 | CB  | VAL | 155 | 22.308 | -17.637 | 38.989 | 1.00 | 0.00 | 3A7 |
| ATOM | 904 | CG1 | VAL | 155 | 23.103 | -16.370 | 38.590 | 1.00 | 0.00 | 3A7 |
| ATOM | 905 | CG2 | VAL | 155 | 23.251 | -18.537 | 39.870 | 1.00 | 0.00 | 3A7 |
| ATOM | 906 | C   | VAL | 155 | 20.273 | -16.247 | 39.005 | 1.00 | 0.00 | 3A7 |
| ATOM | 907 | O   | VAL | 155 | 20.407 | -15.062 | 39.286 | 1.00 | 0.00 | 3A7 |
| ATOM | 908 | N   | LEU | 156 | 19.427 | -16.653 | 38.035 | 1.00 | 0.00 | 3A7 |
| ATOM | 909 | CA  | LEU | 156 | 18.566 | -15.759 | 37.295 | 1.00 | 0.00 | 3A7 |
| ATOM | 910 | CB  | LEU | 156 | 17.791 | -16.496 | 36.208 | 1.00 | 0.00 | 3A7 |
| ATOM | 911 | CG  | LEU | 156 | 17.040 | -15.502 | 35.295 | 1.00 | 0.00 | 3A7 |
| ATOM | 912 | CD1 | LEU | 156 | 17.539 | -15.527 | 33.841 | 1.00 | 0.00 | 3A7 |
| ATOM | 913 | CD2 | LEU | 156 | 15.520 | -15.740 | 35.345 | 1.00 | 0.00 | 3A7 |
| ATOM | 914 | C   | LEU | 156 | 17.570 | -15.040 | 38.134 | 1.00 | 0.00 | 3A7 |
| ATOM | 915 | O   | LEU | 156 | 17.442 | -13.817 | 38.081 | 1.00 | 0.00 | 3A7 |
| ATOM | 916 | N   | VAL | 157 | 16.840 | -15.805 | 38.969 | 1.00 | 0.00 | 3A7 |
| ATOM | 917 | CA  | VAL | 157 | 15.830 | -15.290 | 39.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 918 | CB  | VAL | 157 | 15.164 | -16.419 | 40.629 | 1.00 | 0.00 | 3A7 |
| ATOM | 919 | CG1 | VAL | 157 | 14.204 | -15.903 | 41.728 | 1.00 | 0.00 | 3A7 |
| ATOM | 920 | CG2 | VAL | 157 | 14.373 | -17.263 | 39.609 | 1.00 | 0.00 | 3A7 |
| ATOM | 921 | C   | VAL | 157 | 16.437 | -14.314 | 40.832 | 1.00 | 0.00 | 3A7 |
| ATOM | 922 | O   | VAL | 157 | 15.906 | -13.236 | 41.069 | 1.00 | 0.00 | 3A7 |
| ATOM | 923 | N   | ARG | 158 | 17.626 | -14.668 | 41.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 924 | CA  | ARG | 158 | 18.365 | -13.822 | 42.251 | 1.00 | 0.00 | 3A7 |
| ATOM | 925 | CB  | ARG | 158 | 19.590 | -14.557 | 42.789 | 1.00 | 0.00 | 3A7 |
| ATOM | 926 | CG  | ARG | 158 | 20.308 | -13.863 | 43.961 | 1.00 | 0.00 | 3A7 |
| ATOM | 927 | CD  | ARG | 158 | 21.475 | -14.689 | 44.519 | 1.00 | 0.00 | 3A7 |
| ATOM | 928 | NE  | ARG | 158 | 20.932 | -15.988 | 45.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 929 | CZ  | ARG | 158 | 21.742 | -17.042 | 45.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 930 | NH1 | ARG | 158 | 21.187 | -18.206 | 45.808 | 1.00 | 0.00 | 3A7 |
| ATOM | 931 | NH2 | ARG | 158 | 23.097 | -16.943 | 45.230 | 1.00 | 0.00 | 3A7 |
| ATOM | 932 | C   | ARG | 158 | 18.810 | -12.537 | 41.638 | 1.00 | 0.00 | 3A7 |
| ATOM | 933 | O   | ARG | 158 | 18.732 | -11.498 | 42.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 934 | N   | ASN | 159 | 19.237 | -12.550 | 40.359 | 1.00 | 0.00 | 3A7 |
| ATOM | 935 | CA  | ASN | 159 | 19.621 | -11.357 | 39.637 | 1.00 | 0.00 | 3A7 |
| ATOM | 936 | CB  | ASN | 159 | 20.171 | -11.697 | 38.250 | 1.00 | 0.00 | 3A7 |
| ATOM | 937 | CG  | ASN | 159 | 21.490 | -12.475 | 38.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 938 | OD1 | ASN | 159 | 22.072 | -12.627 | 39.439 | 1.00 | 0.00 | 3A7 |
| ATOM | 939 | ND2 | ASN | 159 | 21.964 | -12.980 | 37.177 | 1.00 | 0.00 | 3A7 |
| ATOM | 940 | C   | ASN | 159 | 18.466 | -10.408 | 39.454 | 1.00 | 0.00 | 3A7 |
| ATOM | 941 | O   | ASN | 159 | 18.606 | -9.195  | 39.568 | 1.00 | 0.00 | 3A7 |
| ATOM | 942 | N   | LEU | 160 | 17.267 | -10.966 | 39.205 | 1.00 | 0.00 | 3A7 |
| ATOM | 943 | CA  | LEU | 160 | 16.066 | -10.198 | 39.031 | 1.00 | 0.00 | 3A7 |
| ATOM | 944 | CB  | LEU | 160 | 14.972 | -11.061 | 38.383 | 1.00 | 0.00 | 3A7 |
| ATOM | 945 | CG  | LEU | 160 | 15.234 | -11.457 | 36.902 | 1.00 | 0.00 | 3A7 |
| ATOM | 946 | CD1 | LEU | 160 | 14.149 | -12.430 | 36.402 | 1.00 | 0.00 | 3A7 |
| ATOM | 947 | CD2 | LEU | 160 | 15.359 | -10.246 | 35.959 | 1.00 | 0.00 | 3A7 |
| ATOM | 948 | C   | LEU | 160 | 15.557 | -9.655  | 40.349 | 1.00 | 0.00 | 3A7 |
| ATOM | 949 | O   | LEU | 160 | 14.965 | -8.580  | 40.420 | 1.00 | 0.00 | 3A7 |
| ATOM | 950 | N   | ARG | 161 | 15.836 | -10.377 | 41.455 | 1.00 | 0.00 | 3A7 |
| ATOM | 951 | CA  | ARG | 161 | 15.487 | -9.958  | 42.787 | 1.00 | 0.00 | 3A7 |
| ATOM | 952 | CB  | ARG | 161 | 15.773 | -11.052 | 43.830 | 1.00 | 0.00 | 3A7 |
| ATOM | 953 | CG  | ARG | 161 | 14.640 | -12.097 | 43.887 | 1.00 | 0.00 | 3A7 |
| ATOM | 954 | CD  | ARG | 161 | 14.752 | -13.097 | 45.047 | 1.00 | 0.00 | 3A7 |
| ATOM | 955 | NE  | ARG | 161 | 15.964 | -13.954 | 44.841 | 1.00 | 0.00 | 3A7 |
| ATOM | 956 | CZ  | ARG | 161 | 16.221 | -15.051 | 45.617 | 1.00 | 0.00 | 3A7 |
| ATOM | 957 | NH1 | ARG | 161 | 17.333 | -15.804 | 45.374 | 1.00 | 0.00 | 3A7 |
| ATOM | 958 | NH2 | ARG | 161 | 15.375 | -15.400 | 46.629 | 1.00 | 0.00 | 3A7 |
| ATOM | 959 | C   | ARG | 161 | 16.228 | -8.712  | 43.210 | 1.00 | 0.00 | 3A7 |
| ATOM | 960 | O   | ARG | 161 | 15.673 | -7.843  | 43.879 | 1.00 | 0.00 | 3A7 |
| ATOM | 961 | N   | ARG | 162 | 17.510 | -8.597  | 42.792 | 1.00 | 0.00 | 3A7 |
| ATOM | 962 | CA  | ARG | 162 | 18.380 | -7.499  | 43.134 | 1.00 | 0.00 | 3A7 |
| ATOM | 963 | CB  | ARG | 162 | 19.851 | -7.869  | 42.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 964 | CG  | ARG | 162 | 20.346 | -8.986  | 43.829 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 965  | CD  | ARG | 162 | 21.838 | -9.302  | 43.666 | 1.00 | 0.00 | 3A7 |
| ATOM | 966  | NE  | ARG | 162 | 22.095 | -9.696  | 42.242 | 1.00 | 0.00 | 3A7 |
| ATOM | 967  | CZ  | ARG | 162 | 23.363 | -9.855  | 41.755 | 1.00 | 0.00 | 3A7 |
| ATOM | 968  | NH1 | ARG | 162 | 23.548 | -10.141 | 40.433 | 1.00 | 0.00 | 3A7 |
| ATOM | 969  | NH2 | ARG | 162 | 24.444 | -9.724  | 42.577 | 1.00 | 0.00 | 3A7 |
| ATOM | 970  | C   | ARG | 162 | 18.080 | -6.236  | 42.355 | 1.00 | 0.00 | 3A7 |
| ATOM | 971  | O   | ARG | 162 | 18.755 | -5.220  | 42.500 | 1.00 | 0.00 | 3A7 |
| ATOM | 972  | N   | GLU | 163 | 17.014 | -6.247  | 41.519 | 1.00 | 0.00 | 3A7 |
| ATOM | 973  | CA  | GLU | 163 | 16.615 | -5.103  | 40.744 | 1.00 | 0.00 | 3A7 |
| ATOM | 974  | CB  | GLU | 163 | 15.965 | -5.504  | 39.413 | 1.00 | 0.00 | 3A7 |
| ATOM | 975  | CG  | GLU | 163 | 16.981 | -6.330  | 38.605 | 1.00 | 0.00 | 3A7 |
| ATOM | 976  | CD  | GLU | 163 | 16.426 | -6.716  | 37.246 | 1.00 | 0.00 | 3A7 |
| ATOM | 977  | OE1 | GLU | 163 | 17.080 | -6.372  | 36.227 | 1.00 | 0.00 | 3A7 |
| ATOM | 978  | OE2 | GLU | 163 | 15.354 | -7.376  | 37.210 | 1.00 | 0.00 | 3A7 |
| ATOM | 979  | C   | GLU | 163 | 15.784 | -4.183  | 41.582 | 1.00 | 0.00 | 3A7 |
| ATOM | 980  | O   | GLU | 163 | 15.662 | -2.998  | 41.288 | 1.00 | 0.00 | 3A7 |
| ATOM | 981  | N   | ALA | 164 | 15.230 | -4.708  | 42.699 | 1.00 | 0.00 | 3A7 |
| ATOM | 982  | CA  | ALA | 164 | 14.728 | -3.939  | 43.812 | 1.00 | 0.00 | 3A7 |
| ATOM | 983  | CB  | ALA | 164 | 15.779 | -2.963  | 44.394 | 1.00 | 0.00 | 3A7 |
| ATOM | 984  | C   | ALA | 164 | 13.480 | -3.200  | 43.529 | 1.00 | 0.00 | 3A7 |
| ATOM | 985  | O   | ALA | 164 | 13.505 | -1.993  | 43.644 | 1.00 | 0.00 | 3A7 |
| ATOM | 986  | N   | GLU | 165 | 12.363 | -3.878  | 43.176 | 1.00 | 0.00 | 3A7 |
| ATOM | 987  | CA  | GLU | 165 | 10.993 | -3.400  | 43.222 | 1.00 | 0.00 | 3A7 |
| ATOM | 988  | CB  | GLU | 165 | 10.561 | -2.688  | 44.540 | 1.00 | 0.00 | 3A7 |
| ATOM | 989  | CG  | GLU | 165 | 10.851 | -3.510  | 45.809 | 1.00 | 0.00 | 3A7 |
| ATOM | 990  | CD  | GLU | 165 | 10.308 | -2.803  | 47.050 | 1.00 | 0.00 | 3A7 |
| ATOM | 991  | OE1 | GLU | 165 | 9.757  | -1.678  | 46.915 | 1.00 | 0.00 | 3A7 |
| ATOM | 992  | OE2 | GLU | 165 | 10.441 | -3.390  | 48.158 | 1.00 | 0.00 | 3A7 |
| ATOM | 993  | C   | GLU | 165 | 10.541 | -2.574  | 42.031 | 1.00 | 0.00 | 3A7 |
| ATOM | 994  | O   | GLU | 165 | 9.403  | -2.728  | 41.595 | 1.00 | 0.00 | 3A7 |
| ATOM | 995  | N   | THR | 166 | 11.382 | -1.661  | 41.488 | 1.00 | 0.00 | 3A7 |
| ATOM | 996  | CA  | THR | 166 | 10.979 | -0.758  | 40.425 | 1.00 | 0.00 | 3A7 |
| ATOM | 997  | CB  | THR | 166 | 10.351 | 0.509   | 40.932 | 1.00 | 0.00 | 3A7 |
| ATOM | 998  | OG1 | THR | 166 | 9.175  | 0.217   | 41.676 | 1.00 | 0.00 | 3A7 |
| ATOM | 999  | CG2 | THR | 166 | 9.944  | 1.442   | 39.767 | 1.00 | 0.00 | 3A7 |
| ATOM | 1000 | C   | THR | 166 | 12.235 | -0.374  | 39.728 | 1.00 | 0.00 | 3A7 |
| ATOM | 1001 | O   | THR | 166 | 12.410 | -0.652  | 38.547 | 1.00 | 0.00 | 3A7 |
| ATOM | 1002 | N   | GLY | 167 | 13.141 | 0.230   | 40.560 | 1.00 | 0.00 | 3A7 |
| ATOM | 1003 | CA  | GLY | 167 | 14.556 | 0.524   | 40.415 | 1.00 | 0.00 | 3A7 |
| ATOM | 1004 | C   | GLY | 167 | 14.980 | 0.965   | 39.058 | 1.00 | 0.00 | 3A7 |
| ATOM | 1005 | O   | GLY | 167 | 15.037 | 2.155   | 38.750 | 1.00 | 0.00 | 3A7 |
| ATOM | 1006 | N   | LYS | 168 | 15.246 | -0.048  | 38.208 | 1.00 | 0.00 | 3A7 |
| ATOM | 1007 | CA  | LYS | 168 | 15.423 | 0.121   | 36.801 | 1.00 | 0.00 | 3A7 |
| ATOM | 1008 | CB  | LYS | 168 | 16.887 | -0.172  | 36.380 | 1.00 | 0.00 | 3A7 |
| ATOM | 1009 | CG  | LYS | 168 | 17.309 | 0.475   | 35.050 | 1.00 | 0.00 | 3A7 |
| ATOM | 1010 | CD  | LYS | 168 | 18.803 | 0.294   | 34.725 | 1.00 | 0.00 | 3A7 |
| ATOM | 1011 | CE  | LYS | 168 | 19.236 | -1.160  | 34.483 | 1.00 | 0.00 | 3A7 |
| ATOM | 1012 | NZ  | LYS | 168 | 18.558 | -1.731  | 33.297 | 1.00 | 0.00 | 3A7 |
| ATOM | 1013 | C   | LYS | 168 | 14.438 | -0.857  | 36.181 | 1.00 | 0.00 | 3A7 |
| ATOM | 1014 | O   | LYS | 168 | 14.315 | -1.969  | 36.694 | 1.00 | 0.00 | 3A7 |
| ATOM | 1015 | N   | PRO | 169 | 13.751 | -0.544  | 35.061 | 1.00 | 0.00 | 3A7 |
| ATOM | 1016 | CA  | PRO | 169 | 13.228 | -1.488  | 34.077 | 1.00 | 0.00 | 3A7 |
| ATOM | 1017 | CD  | PRO | 169 | 13.706 | 0.834   | 34.565 | 1.00 | 0.00 | 3A7 |
| ATOM | 1018 | CB  | PRO | 169 | 12.639 | -0.568  | 33.005 | 1.00 | 0.00 | 3A7 |
| ATOM | 1019 | CG  | PRO | 169 | 13.438 | 0.725   | 33.072 | 1.00 | 0.00 | 3A7 |
| ATOM | 1020 | C   | PRO | 169 | 14.386 | -2.289  | 33.508 | 1.00 | 0.00 | 3A7 |
| ATOM | 1021 | O   | PRO | 169 | 15.533 | -1.866  | 33.608 | 1.00 | 0.00 | 3A7 |
| ATOM | 1022 | N   | VAL | 170 | 14.110 | -3.480  | 32.963 | 1.00 | 0.00 | 3A7 |
| ATOM | 1023 | CA  | VAL | 170 | 15.120 | -4.462  | 32.688 | 1.00 | 0.00 | 3A7 |
| ATOM | 1024 | CB  | VAL | 170 | 14.791 | -5.773  | 33.379 | 1.00 | 0.00 | 3A7 |
| ATOM | 1025 | CG1 | VAL | 170 | 15.992 | -6.742  | 33.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 1026 | CG2 | VAL | 170 | 14.350 | -5.485  | 34.825 | 1.00 | 0.00 | 3A7 |
| ATOM | 1027 | C   | VAL | 170 | 15.190 | -4.659  | 31.200 | 1.00 | 0.00 | 3A7 |
| ATOM | 1028 | O   | VAL | 170 | 14.185 | -4.556  | 30.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 1029 | N   | THR | 171 | 16.400 | -4.984  | 30.690 | 1.00 | 0.00 | 3A7 |
| ATOM | 1030 | CA  | THR | 171 | 16.616 | -5.364  | 29.321 | 1.00 | 0.00 | 3A7 |
| ATOM | 1031 | CB  | THR | 171 | 17.889 | -4.784  | 28.730 | 1.00 | 0.00 | 3A7 |
| ATOM | 1032 | OG1 | THR | 171 | 17.858 | -3.368  | 28.857 | 1.00 | 0.00 | 3A7 |
| ATOM | 1033 | CG2 | THR | 171 | 18.018 | -5.145  | 27.233 | 1.00 | 0.00 | 3A7 |
| ATOM | 1034 | C   | THR | 171 | 16.717 | -6.854  | 29.319 | 1.00 | 0.00 | 3A7 |
| ATOM | 1035 | O   | THR | 171 | 17.667 | -7.434  | 29.839 | 1.00 | 0.00 | 3A7 |
| ATOM | 1036 | N   | LEU | 172 | 15.716 | -7.527  | 28.719 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1037 | CA  | LEU | 172 | 15.566 | -8.955  | 28.820 | 1.00 | 0.00 | 3A7 |
| ATOM | 1038 | CB  | LEU | 172 | 14.147 | -9.409  | 28.421 | 1.00 | 0.00 | 3A7 |
| ATOM | 1039 | CG  | LEU | 172 | 12.958 | -8.735  | 29.139 | 1.00 | 0.00 | 3A7 |
| ATOM | 1040 | CD1 | LEU | 172 | 13.118 | -8.664  | 30.670 | 1.00 | 0.00 | 3A7 |
| ATOM | 1041 | CD2 | LEU | 172 | 12.633 | -7.378  | 28.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 1042 | C   | LEU | 172 | 16.574 | -9.705  | 27.991 | 1.00 | 0.00 | 3A7 |
| ATOM | 1043 | O   | LEU | 172 | 17.033 | -10.771 | 28.384 | 1.00 | 0.00 | 3A7 |
| ATOM | 1044 | N   | LYS | 173 | 16.994 | -9.161  | 26.826 | 1.00 | 0.00 | 3A7 |
| ATOM | 1045 | CA  | LYS | 173 | 17.961 | -9.803  | 25.952 | 1.00 | 0.00 | 3A7 |
| ATOM | 1046 | CB  | LYS | 173 | 18.202 | -8.967  | 24.685 | 1.00 | 0.00 | 3A7 |
| ATOM | 1047 | CG  | LYS | 173 | 19.033 | -9.687  | 23.605 | 1.00 | 0.00 | 3A7 |
| ATOM | 1048 | CD  | LYS | 173 | 19.257 | -8.825  | 22.357 | 1.00 | 0.00 | 3A7 |
| ATOM | 1049 | CE  | LYS | 173 | 19.931 | -9.589  | 21.211 | 1.00 | 0.00 | 3A7 |
| ATOM | 1050 | NZ  | LYS | 173 | 20.065 | -8.725  | 20.017 | 1.00 | 0.00 | 3A7 |
| ATOM | 1051 | C   | LYS | 173 | 19.296 | -10.057 | 26.620 | 1.00 | 0.00 | 3A7 |
| ATOM | 1052 | O   | LYS | 173 | 19.912 | -11.106 | 26.445 | 1.00 | 0.00 | 3A7 |
| ATOM | 1053 | N   | HIS | 174 | 19.729 | -9.103  | 27.472 | 1.00 | 0.00 | 3A7 |
| ATOM | 1054 | CA  | HIS | 174 | 20.962 | -9.190  | 28.204 | 1.00 | 0.00 | 3A7 |
| ATOM | 1055 | ND1 | HIS | 174 | 23.840 | -7.893  | 28.844 | 1.00 | 0.00 | 3A7 |
| ATOM | 1056 | CG  | HIS | 174 | 22.644 | -7.783  | 29.521 | 1.00 | 0.00 | 3A7 |
| ATOM | 1057 | CB  | HIS | 174 | 21.288 | -7.846  | 28.865 | 1.00 | 0.00 | 3A7 |
| ATOM | 1058 | NE2 | HIS | 174 | 24.347 | -7.664  | 30.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 1059 | CD2 | HIS | 174 | 22.973 | -7.645  | 30.834 | 1.00 | 0.00 | 3A7 |
| ATOM | 1060 | CE1 | HIS | 174 | 24.824 | -7.814  | 29.775 | 1.00 | 0.00 | 3A7 |
| ATOM | 1061 | C   | HIS | 174 | 20.970 | -10.255 | 29.275 | 1.00 | 0.00 | 3A7 |
| ATOM | 1062 | O   | HIS | 174 | 21.877 | -11.082 | 29.317 | 1.00 | 0.00 | 3A7 |
| ATOM | 1063 | N   | VAL | 175 | 19.954 | -10.272 | 30.170 | 1.00 | 0.00 | 3A7 |
| ATOM | 1064 | CA  | VAL | 175 | 19.876 | -11.181 | 31.303 | 1.00 | 0.00 | 3A7 |
| ATOM | 1065 | CB  | VAL | 175 | 18.832 | -10.715 | 32.291 | 1.00 | 0.00 | 3A7 |
| ATOM | 1066 | CG1 | VAL | 175 | 18.836 | -11.586 | 33.568 | 1.00 | 0.00 | 3A7 |
| ATOM | 1067 | CG2 | VAL | 175 | 19.117 | -9.239  | 32.645 | 1.00 | 0.00 | 3A7 |
| ATOM | 1068 | C   | VAL | 175 | 19.575 | -12.603 | 30.872 | 1.00 | 0.00 | 3A7 |
| ATOM | 1069 | O   | VAL | 175 | 20.055 | -13.576 | 31.455 | 1.00 | 0.00 | 3A7 |
| ATOM | 1070 | N   | PHE | 176 | 18.769 | -12.751 | 29.799 | 1.00 | 0.00 | 3A7 |
| ATOM | 1071 | CA  | PHE | 176 | 18.383 | -14.047 | 29.302 | 1.00 | 0.00 | 3A7 |
| ATOM | 1072 | CB  | PHE | 176 | 17.044 | -13.978 | 28.573 | 1.00 | 0.00 | 3A7 |
| ATOM | 1073 | CG  | PHE | 176 | 15.984 | -14.019 | 29.651 | 1.00 | 0.00 | 3A7 |
| ATOM | 1074 | CD1 | PHE | 176 | 15.271 | -12.887 | 30.048 | 1.00 | 0.00 | 3A7 |
| ATOM | 1075 | CD2 | PHE | 176 | 15.760 | -15.216 | 30.337 | 1.00 | 0.00 | 3A7 |
| ATOM | 1076 | CE1 | PHE | 176 | 14.380 | -12.941 | 31.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 1077 | CE2 | PHE | 176 | 14.857 | -15.282 | 31.394 | 1.00 | 0.00 | 3A7 |
| ATOM | 1078 | CZ  | PHE | 176 | 14.171 | -14.139 | 31.790 | 1.00 | 0.00 | 3A7 |
| ATOM | 1079 | C   | PHE | 176 | 19.411 | -14.648 | 28.382 | 1.00 | 0.00 | 3A7 |
| ATOM | 1080 | O   | PHE | 176 | 19.429 | -15.860 | 28.180 | 1.00 | 0.00 | 3A7 |
| ATOM | 1081 | N   | GLY | 177 | 20.328 | -13.824 | 27.829 | 1.00 | 0.00 | 3A7 |
| ATOM | 1082 | CA  | GLY | 177 | 21.447 | -14.314 | 27.061 | 1.00 | 0.00 | 3A7 |
| ATOM | 1083 | C   | GLY | 177 | 22.530 | -14.791 | 27.997 | 1.00 | 0.00 | 3A7 |
| ATOM | 1084 | O   | GLY | 177 | 23.231 | -15.756 | 27.714 | 1.00 | 0.00 | 3A7 |
| ATOM | 1085 | N   | ALA | 178 | 22.657 | -14.142 | 29.180 | 1.00 | 0.00 | 3A7 |
| ATOM | 1086 | CA  | ALA | 178 | 23.616 | -14.483 | 30.214 | 1.00 | 0.00 | 3A7 |
| ATOM | 1087 | CB  | ALA | 178 | 23.639 | -13.426 | 31.327 | 1.00 | 0.00 | 3A7 |
| ATOM | 1088 | C   | ALA | 178 | 23.303 | -15.805 | 30.855 | 1.00 | 0.00 | 3A7 |
| ATOM | 1089 | O   | ALA | 178 | 24.178 | -16.635 | 31.070 | 1.00 | 0.00 | 3A7 |
| ATOM | 1090 | N   | TYR | 179 | 22.004 | -16.063 | 31.127 | 1.00 | 0.00 | 3A7 |
| ATOM | 1091 | CA  | TYR | 179 | 21.522 | -17.288 | 31.732 | 1.00 | 0.00 | 3A7 |
| ATOM | 1092 | CB  | TYR | 179 | 19.979 | -17.174 | 31.929 | 1.00 | 0.00 | 3A7 |
| ATOM | 1093 | CG  | TYR | 179 | 19.104 | -18.432 | 31.952 | 1.00 | 0.00 | 3A7 |
| ATOM | 1094 | CD1 | TYR | 179 | 18.538 | -18.892 | 33.140 | 1.00 | 0.00 | 3A7 |
| ATOM | 1095 | CD2 | TYR | 179 | 18.795 | -19.133 | 30.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 1096 | CE1 | TYR | 179 | 17.873 | -20.112 | 33.200 | 1.00 | 0.00 | 3A7 |
| ATOM | 1097 | CE2 | TYR | 179 | 18.128 | -20.354 | 30.824 | 1.00 | 0.00 | 3A7 |
| ATOM | 1098 | CZ  | TYR | 179 | 17.709 | -20.868 | 32.046 | 1.00 | 0.00 | 3A7 |
| ATOM | 1099 | OH  | TYR | 179 | 17.108 | -22.143 | 32.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 1100 | C   | TYR | 179 | 21.881 | -18.504 | 30.914 | 1.00 | 0.00 | 3A7 |
| ATOM | 1101 | O   | TYR | 179 | 22.420 | -19.487 | 31.413 | 1.00 | 0.00 | 3A7 |
| ATOM | 1102 | N   | SER | 180 | 21.607 | -18.432 | 29.602 | 1.00 | 0.00 | 3A7 |
| ATOM | 1103 | CA  | SER | 180 | 21.758 | -19.553 | 28.719 | 1.00 | 0.00 | 3A7 |
| ATOM | 1104 | CB  | SER | 180 | 20.943 | -19.328 | 27.464 | 1.00 | 0.00 | 3A7 |
| ATOM | 1105 | OG  | SER | 180 | 21.331 | -18.109 | 26.860 | 1.00 | 0.00 | 3A7 |
| ATOM | 1106 | C   | SER | 180 | 23.198 | -19.852 | 28.402 | 1.00 | 0.00 | 3A7 |
| ATOM | 1107 | O   | SER | 180 | 23.565 | -21.010 | 28.278 | 1.00 | 0.00 | 3A7 |
| ATOM | 1108 | N   | MET | 181 | 24.084 | -18.834 | 28.319 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1109 | CA  | MET | 181 | 25.507 | -19.052 | 28.132 | 1.00 | 0.00 | 3A7 |
| ATOM | 1110 | CB  | MET | 181 | 26.246 | -17.722 | 27.978 | 1.00 | 0.00 | 3A7 |
| ATOM | 1111 | CG  | MET | 181 | 25.986 | -17.169 | 26.568 | 1.00 | 0.00 | 3A7 |
| ATOM | 1112 | SD  | MET | 181 | 26.894 | -15.667 | 26.130 | 1.00 | 0.00 | 3A7 |
| ATOM | 1113 | CE  | MET | 181 | 25.919 | -14.578 | 27.203 | 1.00 | 0.00 | 3A7 |
| ATOM | 1114 | C   | MET | 181 | 26.127 | -19.780 | 29.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 1115 | O   | MET | 181 | 26.923 | -20.700 | 29.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 1116 | N   | ASP | 182 | 25.695 | -19.407 | 30.493 | 1.00 | 0.00 | 3A7 |
| ATOM | 1117 | CA  | ASP | 182 | 26.174 | -20.008 | 31.695 | 1.00 | 0.00 | 3A7 |
| ATOM | 1118 | CB  | ASP | 182 | 25.809 | -19.160 | 32.908 | 1.00 | 0.00 | 3A7 |
| ATOM | 1119 | CG  | ASP | 182 | 26.545 | -17.813 | 32.877 | 1.00 | 0.00 | 3A7 |
| ATOM | 1120 | OD1 | ASP | 182 | 27.380 | -17.590 | 31.961 | 1.00 | 0.00 | 3A7 |
| ATOM | 1121 | OD2 | ASP | 182 | 26.276 | -16.986 | 33.788 | 1.00 | 0.00 | 3A7 |
| ATOM | 1122 | C   | ASP | 182 | 25.645 | -21.408 | 31.886 | 1.00 | 0.00 | 3A7 |
| ATOM | 1123 | O   | ASP | 182 | 26.371 | -22.258 | 32.382 | 1.00 | 0.00 | 3A7 |
| ATOM | 1124 | N   | VAL | 183 | 24.401 | -21.724 | 31.448 | 1.00 | 0.00 | 3A7 |
| ATOM | 1125 | CA  | VAL | 183 | 23.887 | -23.084 | 31.514 | 1.00 | 0.00 | 3A7 |
| ATOM | 1126 | CB  | VAL | 183 | 22.419 | -23.173 | 31.124 | 1.00 | 0.00 | 3A7 |
| ATOM | 1127 | CG1 | VAL | 183 | 21.919 | -24.632 | 30.984 | 1.00 | 0.00 | 3A7 |
| ATOM | 1128 | CG2 | VAL | 183 | 21.578 | -22.468 | 32.200 | 1.00 | 0.00 | 3A7 |
| ATOM | 1129 | C   | VAL | 183 | 24.678 | -24.016 | 30.610 | 1.00 | 0.00 | 3A7 |
| ATOM | 1130 | O   | VAL | 183 | 25.065 | -25.103 | 31.027 | 1.00 | 0.00 | 3A7 |
| ATOM | 1131 | N   | ILE | 184 | 24.999 | -23.597 | 29.353 | 1.00 | 0.00 | 3A7 |
| ATOM | 1132 | CA  | ILE | 184 | 25.762 | -24.395 | 28.439 | 1.00 | 0.00 | 3A7 |
| ATOM | 1133 | CB  | ILE | 184 | 25.800 | -23.816 | 27.039 | 1.00 | 0.00 | 3A7 |
| ATOM | 1134 | CG2 | ILE | 184 | 26.594 | -24.750 | 26.093 | 1.00 | 0.00 | 3A7 |
| ATOM | 1135 | CG1 | ILE | 184 | 24.365 | -23.617 | 26.489 | 1.00 | 0.00 | 3A7 |
| ATOM | 1136 | CD  | ILE | 184 | 23.531 | -24.898 | 26.404 | 1.00 | 0.00 | 3A7 |
| ATOM | 1137 | C   | ILE | 184 | 27.167 | -24.561 | 28.928 | 1.00 | 0.00 | 3A7 |
| ATOM | 1138 | O   | ILE | 184 | 27.720 | -25.652 | 28.859 | 1.00 | 0.00 | 3A7 |
| ATOM | 1139 | N   | THR | 185 | 27.774 | -23.489 | 29.486 | 1.00 | 0.00 | 3A7 |
| ATOM | 1140 | CA  | THR | 185 | 29.125 | -23.511 | 30.002 | 1.00 | 0.00 | 3A7 |
| ATOM | 1141 | CB  | THR | 185 | 29.617 | -22.111 | 30.359 | 1.00 | 0.00 | 3A7 |
| ATOM | 1142 | OG1 | THR | 185 | 29.625 | -21.307 | 29.187 | 1.00 | 0.00 | 3A7 |
| ATOM | 1143 | CG2 | THR | 185 | 31.047 | -22.108 | 30.943 | 1.00 | 0.00 | 3A7 |
| ATOM | 1144 | C   | THR | 185 | 29.259 | -24.418 | 31.192 | 1.00 | 0.00 | 3A7 |
| ATOM | 1145 | O   | THR | 185 | 30.220 | -25.166 | 31.343 | 1.00 | 0.00 | 3A7 |
| ATOM | 1146 | N   | SER | 186 | 28.242 | -24.404 | 32.066 | 1.00 | 0.00 | 3A7 |
| ATOM | 1147 | CA  | SER | 186 | 28.262 | -25.188 | 33.262 | 1.00 | 0.00 | 3A7 |
| ATOM | 1148 | CB  | SER | 186 | 27.223 | -24.719 | 34.259 | 1.00 | 0.00 | 3A7 |
| ATOM | 1149 | OG  | SER | 186 | 27.539 | -23.412 | 34.719 | 1.00 | 0.00 | 3A7 |
| ATOM | 1150 | C   | SER | 186 | 28.037 | -26.655 | 33.000 | 1.00 | 0.00 | 3A7 |
| ATOM | 1151 | O   | SER | 186 | 28.693 | -27.500 | 33.598 | 1.00 | 0.00 | 3A7 |
| ATOM | 1152 | N   | THR | 187 | 27.128 | -27.006 | 32.060 | 1.00 | 0.00 | 3A7 |
| ATOM | 1153 | CA  | THR | 187 | 26.865 | -28.386 | 31.711 | 1.00 | 0.00 | 3A7 |
| ATOM | 1154 | CB  | THR | 187 | 25.561 | -28.580 | 30.943 | 1.00 | 0.00 | 3A7 |
| ATOM | 1155 | OG1 | THR | 187 | 25.480 | -27.748 | 29.789 | 1.00 | 0.00 | 3A7 |
| ATOM | 1156 | CG2 | THR | 187 | 24.359 | -28.285 | 31.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 1157 | C   | THR | 187 | 27.994 | -28.983 | 30.897 | 1.00 | 0.00 | 3A7 |
| ATOM | 1158 | O   | THR | 187 | 28.202 | -30.195 | 30.899 | 1.00 | 0.00 | 3A7 |
| ATOM | 1159 | N   | SER | 188 | 28.739 | -28.115 | 30.176 | 1.00 | 0.00 | 3A7 |
| ATOM | 1160 | CA  | SER | 188 | 29.767 | -28.556 | 29.280 | 1.00 | 0.00 | 3A7 |
| ATOM | 1161 | CB  | SER | 188 | 29.905 | -27.697 | 27.991 | 1.00 | 0.00 | 3A7 |
| ATOM | 1162 | OG  | SER | 188 | 30.272 | -26.347 | 28.250 | 1.00 | 0.00 | 3A7 |
| ATOM | 1163 | C   | SER | 188 | 31.105 | -28.690 | 29.970 | 1.00 | 0.00 | 3A7 |
| ATOM | 1164 | O   | SER | 188 | 31.803 | -29.681 | 29.768 | 1.00 | 0.00 | 3A7 |
| ATOM | 1165 | N   | PHE | 189 | 31.513 | -27.672 | 30.766 | 1.00 | 0.00 | 3A7 |
| ATOM | 1166 | CA  | PHE | 189 | 32.870 | -27.581 | 31.256 | 1.00 | 0.00 | 3A7 |
| ATOM | 1167 | CB  | PHE | 189 | 33.653 | -26.363 | 30.732 | 1.00 | 0.00 | 3A7 |
| ATOM | 1168 | CG  | PHE | 189 | 33.446 | -26.027 | 29.300 | 1.00 | 0.00 | 3A7 |
| ATOM | 1169 | CD1 | PHE | 189 | 33.204 | -24.694 | 28.976 | 1.00 | 0.00 | 3A7 |
| ATOM | 1170 | CD2 | PHE | 189 | 33.468 | -26.986 | 28.292 | 1.00 | 0.00 | 3A7 |
| ATOM | 1171 | CE1 | PHE | 189 | 32.971 | -24.317 | 27.665 | 1.00 | 0.00 | 3A7 |
| ATOM | 1172 | CE2 | PHE | 189 | 33.182 | -26.618 | 26.984 | 1.00 | 0.00 | 3A7 |
| ATOM | 1173 | CZ  | PHE | 189 | 32.933 | -25.284 | 26.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 1174 | C   | PHE | 189 | 32.919 | -27.463 | 32.762 | 1.00 | 0.00 | 3A7 |
| ATOM | 1175 | O   | PHE | 189 | 33.993 | -27.441 | 33.361 | 1.00 | 0.00 | 3A7 |
| ATOM | 1176 | N   | GLY | 190 | 31.743 | -27.378 | 33.435 | 1.00 | 0.00 | 3A7 |
| ATOM | 1177 | CA  | GLY | 190 | 31.654 | -27.345 | 34.883 | 1.00 | 0.00 | 3A7 |
| ATOM | 1178 | C   | GLY | 190 | 31.869 | -25.956 | 35.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 1179 | O   | GLY | 190 | 31.005 | -25.095 | 35.280 | 1.00 | 0.00 | 3A7 |
| ATOM | 1180 | N   | VAL | 191 | 33.057 | -25.744 | 36.044 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1181 | CA  | VAL | 191 | 33.597 | -24.510 | 36.596 | 1.00 | 0.00 | 3A7 |
| ATOM | 1182 | CB  | VAL | 191 | 33.426 | -23.250 | 35.727 | 1.00 | 0.00 | 3A7 |
| ATOM | 1183 | CG1 | VAL | 191 | 32.199 | -22.372 | 36.078 | 1.00 | 0.00 | 3A7 |
| ATOM | 1184 | CG2 | VAL | 191 | 34.729 | -22.424 | 35.812 | 1.00 | 0.00 | 3A7 |
| ATOM | 1185 | C   | VAL | 191 | 33.100 | -24.310 | 38.012 | 1.00 | 0.00 | 3A7 |
| ATOM | 1186 | O   | VAL | 191 | 31.935 | -24.551 | 38.325 | 1.00 | 0.00 | 3A7 |
| ATOM | 1187 | N   | SER | 192 | 34.012 | -23.844 | 38.900 | 1.00 | 0.00 | 3A7 |
| ATOM | 1188 | CA  | SER | 192 | 33.727 | -23.531 | 40.281 | 1.00 | 0.00 | 3A7 |
| ATOM | 1189 | CB  | SER | 192 | 34.779 | -24.116 | 41.252 | 1.00 | 0.00 | 3A7 |
| ATOM | 1190 | OG  | SER | 192 | 34.799 | -25.534 | 41.156 | 1.00 | 0.00 | 3A7 |
| ATOM | 1191 | C   | SER | 192 | 33.716 | -22.032 | 40.410 | 1.00 | 0.00 | 3A7 |
| ATOM | 1192 | O   | SER | 192 | 34.136 | -21.317 | 39.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 1193 | N   | ILE | 193 | 33.230 | -21.524 | 41.572 | 1.00 | 0.00 | 3A7 |
| ATOM | 1194 | CA  | ILE | 193 | 33.138 | -20.109 | 41.867 | 1.00 | 0.00 | 3A7 |
| ATOM | 1195 | CB  | ILE | 193 | 31.890 | -19.756 | 42.671 | 1.00 | 0.00 | 3A7 |
| ATOM | 1196 | CG2 | ILE | 193 | 31.794 | -18.225 | 42.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 1197 | CG1 | ILE | 193 | 30.615 | -20.322 | 41.992 | 1.00 | 0.00 | 3A7 |
| ATOM | 1198 | CD  | ILE | 193 | 30.351 | -19.784 | 40.581 | 1.00 | 0.00 | 3A7 |
| ATOM | 1199 | C   | ILE | 193 | 34.389 | -19.720 | 42.618 | 1.00 | 0.00 | 3A7 |
| ATOM | 1200 | O   | ILE | 193 | 34.518 | -19.967 | 43.816 | 1.00 | 0.00 | 3A7 |
| ATOM | 1201 | N   | ASP | 194 | 35.344 | -19.102 | 41.887 | 1.00 | 0.00 | 3A7 |
| ATOM | 1202 | CA  | ASP | 194 | 36.617 | -18.685 | 42.420 | 1.00 | 0.00 | 3A7 |
| ATOM | 1203 | CB  | ASP | 194 | 37.706 | -19.786 | 42.267 | 1.00 | 0.00 | 3A7 |
| ATOM | 1204 | CG  | ASP | 194 | 38.984 | -19.433 | 43.034 | 1.00 | 0.00 | 3A7 |
| ATOM | 1205 | OD1 | ASP | 194 | 38.899 | -19.270 | 44.280 | 1.00 | 0.00 | 3A7 |
| ATOM | 1206 | OD2 | ASP | 194 | 40.056 | -19.326 | 42.381 | 1.00 | 0.00 | 3A7 |
| ATOM | 1207 | C   | ASP | 194 | 36.993 | -17.442 | 41.654 | 1.00 | 0.00 | 3A7 |
| ATOM | 1208 | O   | ASP | 194 | 37.756 | -16.608 | 42.141 | 1.00 | 0.00 | 3A7 |
| ATOM | 1209 | N   | SER | 195 | 36.443 | -17.299 | 40.420 | 1.00 | 0.00 | 3A7 |
| ATOM | 1210 | CA  | SER | 195 | 36.648 | -16.163 | 39.548 | 1.00 | 0.00 | 3A7 |
| ATOM | 1211 | CB  | SER | 195 | 36.679 | -16.561 | 38.055 | 1.00 | 0.00 | 3A7 |
| ATOM | 1212 | OG  | SER | 195 | 37.748 | -17.464 | 37.811 | 1.00 | 0.00 | 3A7 |
| ATOM | 1213 | C   | SER | 195 | 35.523 | -15.185 | 39.763 | 1.00 | 0.00 | 3A7 |
| ATOM | 1214 | O   | SER | 195 | 34.456 | -15.547 | 40.256 | 1.00 | 0.00 | 3A7 |
| ATOM | 1215 | N   | LEU | 196 | 35.759 | -13.902 | 39.386 | 1.00 | 0.00 | 3A7 |
| ATOM | 1216 | CA  | LEU | 196 | 34.826 | -12.813 | 39.580 | 1.00 | 0.00 | 3A7 |
| ATOM | 1217 | CB  | LEU | 196 | 35.494 | -11.523 | 40.138 | 1.00 | 0.00 | 3A7 |
| ATOM | 1218 | CG  | LEU | 196 | 36.127 | -11.639 | 41.551 | 1.00 | 0.00 | 3A7 |
| ATOM | 1219 | CD1 | LEU | 196 | 35.140 | -12.190 | 42.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 1220 | CD2 | LEU | 196 | 37.469 | -12.399 | 41.574 | 1.00 | 0.00 | 3A7 |
| ATOM | 1221 | C   | LEU | 196 | 34.175 | -12.481 | 38.258 | 1.00 | 0.00 | 3A7 |
| ATOM | 1222 | O   | LEU | 196 | 33.796 | -11.334 | 38.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 1223 | N   | ASN | 197 | 34.036 | -13.503 | 37.366 | 1.00 | 0.00 | 3A7 |
| ATOM | 1224 | CA  | ASN | 197 | 33.382 | -13.455 | 36.068 | 1.00 | 0.00 | 3A7 |
| ATOM | 1225 | CB  | ASN | 197 | 31.946 | -12.846 | 36.138 | 1.00 | 0.00 | 3A7 |
| ATOM | 1226 | CG  | ASN | 197 | 31.125 | -13.111 | 34.865 | 1.00 | 0.00 | 3A7 |
| ATOM | 1227 | OD1 | ASN | 197 | 31.170 | -14.206 | 34.295 | 1.00 | 0.00 | 3A7 |
| ATOM | 1228 | ND2 | ASN | 197 | 30.353 | -12.069 | 34.431 | 1.00 | 0.00 | 3A7 |
| ATOM | 1229 | C   | ASN | 197 | 34.255 | -12.714 | 35.072 | 1.00 | 0.00 | 3A7 |
| ATOM | 1230 | O   | ASN | 197 | 33.812 | -11.770 | 34.419 | 1.00 | 0.00 | 3A7 |
| ATOM | 1231 | N   | ASN | 198 | 35.541 | -13.134 | 34.960 | 1.00 | 0.00 | 3A7 |
| ATOM | 1232 | CA  | ASN | 198 | 36.520 | -12.476 | 34.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 1233 | CB  | ASN | 198 | 37.878 | -12.191 | 34.815 | 1.00 | 0.00 | 3A7 |
| ATOM | 1234 | CG  | ASN | 198 | 37.631 | -11.423 | 36.121 | 1.00 | 0.00 | 3A7 |
| ATOM | 1235 | OD1 | ASN | 198 | 37.872 | -11.949 | 37.214 | 1.00 | 0.00 | 3A7 |
| ATOM | 1236 | ND2 | ASN | 198 | 37.143 | -10.153 | 35.986 | 1.00 | 0.00 | 3A7 |
| ATOM | 1237 | C   | ASN | 198 | 36.725 | -13.246 | 32.825 | 1.00 | 0.00 | 3A7 |
| ATOM | 1238 | O   | ASN | 198 | 36.624 | -12.598 | 31.789 | 1.00 | 0.00 | 3A7 |
| ATOM | 1239 | N   | PRO | 199 | 36.993 | -14.562 | 32.735 | 1.00 | 0.00 | 3A7 |
| ATOM | 1240 | CA  | PRO | 199 | 37.251 | -15.242 | 31.473 | 1.00 | 0.00 | 3A7 |
| ATOM | 1241 | CD  | PRO | 199 | 37.339 | -15.415 | 33.865 | 1.00 | 0.00 | 3A7 |
| ATOM | 1242 | CB  | PRO | 199 | 37.966 | -16.553 | 31.866 | 1.00 | 0.00 | 3A7 |
| ATOM | 1243 | CG  | PRO | 199 | 38.421 | -16.338 | 33.313 | 1.00 | 0.00 | 3A7 |
| ATOM | 1244 | C   | PRO | 199 | 35.959 | -15.538 | 30.731 | 1.00 | 0.00 | 3A7 |
| ATOM | 1245 | O   | PRO | 199 | 36.016 | -15.766 | 29.524 | 1.00 | 0.00 | 3A7 |
| ATOM | 1246 | N   | GLN | 200 | 34.800 | -15.560 | 31.441 | 1.00 | 0.00 | 3A7 |
| ATOM | 1247 | CA  | GLN | 200 | 33.519 | -15.967 | 30.914 | 1.00 | 0.00 | 3A7 |
| ATOM | 1248 | CB  | GLN | 200 | 32.614 | -16.559 | 32.023 | 1.00 | 0.00 | 3A7 |
| ATOM | 1249 | CG  | GLN | 200 | 31.297 | -17.173 | 31.515 | 1.00 | 0.00 | 3A7 |
| ATOM | 1250 | CD  | GLN | 200 | 30.581 | -17.885 | 32.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 1251 | OE1 | GLN | 200 | 30.411 | -19.110 | 32.645 | 1.00 | 0.00 | 3A7 |
| ATOM | 1252 | NE2 | GLN | 200 | 30.150 | -17.085 | 33.690 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1253 | C   | GLN | 200 | 32.815 | -14.819 | 30.232 | 1.00 | 0.00 | 3A7 |
| ATOM | 1254 | O   | GLN | 200 | 32.140 | -15.035 | 29.233 | 1.00 | 0.00 | 3A7 |
| ATOM | 1255 | N   | ASP | 201 | 32.961 | -13.568 | 30.743 | 1.00 | 0.00 | 3A7 |
| ATOM | 1256 | CA  | ASP | 201 | 32.288 | -12.384 | 30.219 | 1.00 | 0.00 | 3A7 |
| ATOM | 1257 | CB  | ASP | 201 | 32.223 | -11.254 | 31.288 | 1.00 | 0.00 | 3A7 |
| ATOM | 1258 | CG  | ASP | 201 | 31.197 | -10.174 | 30.927 | 1.00 | 0.00 | 3A7 |
| ATOM | 1259 | OD1 | ASP | 201 | 31.610 | -8.994  | 30.772 | 1.00 | 0.00 | 3A7 |
| ATOM | 1260 | OD2 | ASP | 201 | 29.992 | -10.520 | 30.805 | 1.00 | 0.00 | 3A7 |
| ATOM | 1261 | C   | ASP | 201 | 32.876 | -11.859 | 28.899 | 1.00 | 0.00 | 3A7 |
| ATOM | 1262 | O   | ASP | 201 | 32.107 | -11.342 | 28.095 | 1.00 | 0.00 | 3A7 |
| ATOM | 1263 | N   | PRO | 202 | 34.177 | -11.966 | 28.590 | 1.00 | 0.00 | 3A7 |
| ATOM | 1264 | CA  | PRO | 202 | 34.768 | -11.731 | 27.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 1265 | CD  | PRO | 202 | 35.191 | -11.898 | 29.612 | 1.00 | 0.00 | 3A7 |
| ATOM | 1266 | CB  | PRO | 202 | 36.280 | -11.790 | 27.543 | 1.00 | 0.00 | 3A7 |
| ATOM | 1267 | CG  | PRO | 202 | 36.411 | -11.259 | 28.958 | 1.00 | 0.00 | 3A7 |
| ATOM | 1268 | C   | PRO | 202 | 34.334 | -12.755 | 26.270 | 1.00 | 0.00 | 3A7 |
| ATOM | 1269 | O   | PRO | 202 | 34.099 | -12.386 | 25.126 | 1.00 | 0.00 | 3A7 |
| ATOM | 1270 | N   | PHE | 203 | 34.165 | -14.041 | 26.662 | 1.00 | 0.00 | 3A7 |
| ATOM | 1271 | CA  | PHE | 203 | 33.692 | -15.113 | 25.807 | 1.00 | 0.00 | 3A7 |
| ATOM | 1272 | CB  | PHE | 203 | 33.533 | -16.402 | 26.628 | 1.00 | 0.00 | 3A7 |
| ATOM | 1273 | CG  | PHE | 203 | 33.530 | -17.655 | 25.800 | 1.00 | 0.00 | 3A7 |
| ATOM | 1274 | CD1 | PHE | 203 | 34.701 | -18.401 | 25.685 | 1.00 | 0.00 | 3A7 |
| ATOM | 1275 | CD2 | PHE | 203 | 32.364 | -18.126 | 25.192 | 1.00 | 0.00 | 3A7 |
| ATOM | 1276 | CE1 | PHE | 203 | 34.713 | -19.599 | 24.981 | 1.00 | 0.00 | 3A7 |
| ATOM | 1277 | CE2 | PHE | 203 | 32.377 | -19.316 | 24.471 | 1.00 | 0.00 | 3A7 |
| ATOM | 1278 | CZ  | PHE | 203 | 33.547 | -20.060 | 24.377 | 1.00 | 0.00 | 3A7 |
| ATOM | 1279 | C   | PHE | 203 | 32.360 | -14.780 | 25.173 | 1.00 | 0.00 | 3A7 |
| ATOM | 1280 | O   | PHE | 203 | 32.125 | -15.040 | 23.999 | 1.00 | 0.00 | 3A7 |
| ATOM | 1281 | N   | VAL | 204 | 31.455 | -14.147 | 25.959 | 1.00 | 0.00 | 3A7 |
| ATOM | 1282 | CA  | VAL | 204 | 30.141 | -13.686 | 25.564 | 1.00 | 0.00 | 3A7 |
| ATOM | 1283 | CB  | VAL | 204 | 29.470 | -12.914 | 26.710 | 1.00 | 0.00 | 3A7 |
| ATOM | 1284 | CG1 | VAL | 204 | 28.141 | -12.240 | 26.286 | 1.00 | 0.00 | 3A7 |
| ATOM | 1285 | CG2 | VAL | 204 | 29.308 | -13.845 | 27.927 | 1.00 | 0.00 | 3A7 |
| ATOM | 1286 | C   | VAL | 204 | 30.210 | -12.702 | 24.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 1287 | O   | VAL | 204 | 29.521 | -12.835 | 23.424 | 1.00 | 0.00 | 3A7 |
| ATOM | 1288 | N   | GLU | 205 | 31.077 | -11.674 | 24.576 | 1.00 | 0.00 | 3A7 |
| ATOM | 1289 | CA  | GLU | 205 | 31.235 | -10.607 | 23.617 | 1.00 | 0.00 | 3A7 |
| ATOM | 1290 | CB  | GLU | 205 | 32.215 | -9.544  | 24.146 | 1.00 | 0.00 | 3A7 |
| ATOM | 1291 | CG  | GLU | 205 | 32.242 | -8.242  | 23.327 | 1.00 | 0.00 | 3A7 |
| ATOM | 1292 | CD  | GLU | 205 | 33.217 | -7.267  | 23.979 | 1.00 | 0.00 | 3A7 |
| ATOM | 1293 | OE1 | GLU | 205 | 32.974 | -6.880  | 25.153 | 1.00 | 0.00 | 3A7 |
| ATOM | 1294 | OE2 | GLU | 205 | 34.219 | -6.896  | 23.310 | 1.00 | 0.00 | 3A7 |
| ATOM | 1295 | C   | GLU | 205 | 31.739 | -11.106 | 22.289 | 1.00 | 0.00 | 3A7 |
| ATOM | 1296 | O   | GLU | 205 | 31.308 | -10.646 | 21.238 | 1.00 | 0.00 | 3A7 |
| ATOM | 1297 | N   | ASN | 206 | 32.629 | -12.123 | 22.316 | 1.00 | 0.00 | 3A7 |
| ATOM | 1298 | CA  | ASN | 206 | 33.175 | -12.741 | 21.134 | 1.00 | 0.00 | 3A7 |
| ATOM | 1299 | CB  | ASN | 206 | 34.358 | -13.657 | 21.467 | 1.00 | 0.00 | 3A7 |
| ATOM | 1300 | CG  | ASN | 206 | 35.509 | -12.819 | 22.025 | 1.00 | 0.00 | 3A7 |
| ATOM | 1301 | OD1 | ASN | 206 | 35.798 | -12.848 | 23.224 | 1.00 | 0.00 | 3A7 |
| ATOM | 1302 | ND2 | ASN | 206 | 36.155 | -12.023 | 21.120 | 1.00 | 0.00 | 3A7 |
| ATOM | 1303 | C   | ASN | 206 | 32.151 | -13.539 | 20.380 | 1.00 | 0.00 | 3A7 |
| ATOM | 1304 | O   | ASN | 206 | 31.976 | -13.337 | 19.182 | 1.00 | 0.00 | 3A7 |
| ATOM | 1305 | N   | THR | 207 | 31.417 | -14.452 | 21.067 | 1.00 | 0.00 | 3A7 |
| ATOM | 1306 | CA  | THR | 207 | 30.406 | -15.301 | 20.464 | 1.00 | 0.00 | 3A7 |
| ATOM | 1307 | CB  | THR | 207 | 29.749 | -16.188 | 21.502 | 1.00 | 0.00 | 3A7 |
| ATOM | 1308 | OG1 | THR | 207 | 30.751 | -16.917 | 22.199 | 1.00 | 0.00 | 3A7 |
| ATOM | 1309 | CG2 | THR | 207 | 28.780 | -17.201 | 20.851 | 1.00 | 0.00 | 3A7 |
| ATOM | 1310 | C   | THR | 207 | 29.346 | -14.492 | 19.768 | 1.00 | 0.00 | 3A7 |
| ATOM | 1311 | O   | THR | 207 | 28.951 | -14.790 | 18.646 | 1.00 | 0.00 | 3A7 |
| ATOM | 1312 | N   | LYS | 208 | 28.929 | -13.379 | 20.411 | 1.00 | 0.00 | 3A7 |
| ATOM | 1313 | CA  | LYS | 208 | 27.951 | -12.459 | 19.890 | 1.00 | 0.00 | 3A7 |
| ATOM | 1314 | CB  | LYS | 208 | 27.604 | -11.413 | 20.954 | 1.00 | 0.00 | 3A7 |
| ATOM | 1315 | CG  | LYS | 208 | 26.398 | -10.524 | 20.601 | 1.00 | 0.00 | 3A7 |
| ATOM | 1316 | CD  | LYS | 208 | 25.914 | -9.608  | 21.741 | 1.00 | 0.00 | 3A7 |
| ATOM | 1317 | CE  | LYS | 208 | 26.801 | -8.383  | 22.018 | 1.00 | 0.00 | 3A7 |
| ATOM | 1318 | NZ  | LYS | 208 | 28.077 | -8.751  | 22.673 | 1.00 | 0.00 | 3A7 |
| ATOM | 1319 | C   | LYS | 208 | 28.389 | -11.760 | 18.619 | 1.00 | 0.00 | 3A7 |
| ATOM | 1320 | O   | LYS | 208 | 27.616 | -11.653 | 17.675 | 1.00 | 0.00 | 3A7 |
| ATOM | 1321 | N   | LYS | 209 | 29.664 | -11.316 | 18.536 | 1.00 | 0.00 | 3A7 |
| ATOM | 1322 | CA  | LYS | 209 | 30.209 | -10.686 | 17.348 | 1.00 | 0.00 | 3A7 |
| ATOM | 1323 | CB  | LYS | 209 | 31.622 | -10.129 | 17.587 | 1.00 | 0.00 | 3A7 |
| ATOM | 1324 | CG  | LYS | 209 | 31.660 | -8.877  | 18.478 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1325 | CD  | LYS | 209 | 33.007 | -8.133  | 18.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 1326 | CE  | LYS | 209 | 34.227 | -8.963  | 18.843 | 1.00 | 0.00 | 3A7 |
| ATOM | 1327 | NZ  | LYS | 209 | 34.144 | -9.343  | 20.270 | 1.00 | 0.00 | 3A7 |
| ATOM | 1328 | C   | LYS | 209 | 30.275 | -11.624 | 16.153 | 1.00 | 0.00 | 3A7 |
| ATOM | 1329 | O   | LYS | 209 | 29.942 | -11.252 | 15.031 | 1.00 | 0.00 | 3A7 |
| ATOM | 1330 | N   | LEU | 210 | 30.662 | -12.901 | 16.376 | 1.00 | 0.00 | 3A7 |
| ATOM | 1331 | CA  | LEU | 210 | 30.592 | -13.968 | 15.391 | 1.00 | 0.00 | 3A7 |
| ATOM | 1332 | CB  | LEU | 210 | 30.985 | -15.328 | 16.011 | 1.00 | 0.00 | 3A7 |
| ATOM | 1333 | CG  | LEU | 210 | 31.127 | -16.622 | 15.108 | 1.00 | 0.00 | 3A7 |
| ATOM | 1334 | CD1 | LEU | 210 | 31.072 | -17.872 | 16.013 | 1.00 | 0.00 | 3A7 |
| ATOM | 1335 | CD2 | LEU | 210 | 30.134 | -16.893 | 13.954 | 1.00 | 0.00 | 3A7 |
| ATOM | 1336 | C   | LEU | 210 | 29.217 | -14.131 | 14.809 | 1.00 | 0.00 | 3A7 |
| ATOM | 1337 | O   | LEU | 210 | 29.056 | -14.197 | 13.595 | 1.00 | 0.00 | 3A7 |
| ATOM | 1338 | N   | LEU | 211 | 28.185 | -14.172 | 15.680 | 1.00 | 0.00 | 3A7 |
| ATOM | 1339 | CA  | LEU | 211 | 26.814 | -14.406 | 15.302 | 1.00 | 0.00 | 3A7 |
| ATOM | 1340 | CB  | LEU | 211 | 25.835 | -14.273 | 16.480 | 1.00 | 0.00 | 3A7 |
| ATOM | 1341 | CG  | LEU | 211 | 26.035 | -15.159 | 17.726 | 1.00 | 0.00 | 3A7 |
| ATOM | 1342 | CD1 | LEU | 211 | 24.820 | -15.056 | 18.669 | 1.00 | 0.00 | 3A7 |
| ATOM | 1343 | CD2 | LEU | 211 | 26.398 | -16.614 | 17.396 | 1.00 | 0.00 | 3A7 |
| ATOM | 1344 | C   | LEU | 211 | 26.271 | -13.442 | 14.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 1345 | O   | LEU | 211 | 25.479 | -13.847 | 13.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 1346 | N   | ARG | 212 | 26.667 | -12.140 | 14.324 | 1.00 | 0.00 | 3A7 |
| ATOM | 1347 | CA  | ARG | 212 | 26.196 | -11.136 | 13.386 | 1.00 | 0.00 | 3A7 |
| ATOM | 1348 | CB  | ARG | 212 | 25.985 | -9.737  | 14.028 | 1.00 | 0.00 | 3A7 |
| ATOM | 1349 | CG  | ARG | 212 | 27.103 | -9.170  | 14.927 | 1.00 | 0.00 | 3A7 |
| ATOM | 1350 | CD  | ARG | 212 | 28.270 | -8.508  | 14.183 | 1.00 | 0.00 | 3A7 |
| ATOM | 1351 | NE  | ARG | 212 | 29.078 | -7.724  | 15.175 | 1.00 | 0.00 | 3A7 |
| ATOM | 1352 | CZ  | ARG | 212 | 30.393 | -7.406  | 14.970 | 1.00 | 0.00 | 3A7 |
| ATOM | 1353 | NH1 | ARG | 212 | 31.075 | -7.901  | 13.898 | 1.00 | 0.00 | 3A7 |
| ATOM | 1354 | NH2 | ARG | 212 | 31.031 | -6.581  | 15.851 | 1.00 | 0.00 | 3A7 |
| ATOM | 1355 | C   | ARG | 212 | 27.097 | -11.091 | 12.169 | 1.00 | 0.00 | 3A7 |
| ATOM | 1356 | O   | ARG | 212 | 28.323 | -11.083 | 12.272 | 1.00 | 0.00 | 3A7 |
| ATOM | 1357 | N   | PHE | 213 | 26.441 | -11.117 | 10.976 | 1.00 | 0.00 | 3A7 |
| ATOM | 1358 | CA  | PHE | 213 | 26.943 | -11.263 | 9.611  | 1.00 | 0.00 | 3A7 |
| ATOM | 1359 | CB  | PHE | 213 | 27.428 | -9.944  | 8.921  | 1.00 | 0.00 | 3A7 |
| ATOM | 1360 | CG  | PHE | 213 | 28.597 | -9.221  | 9.541  | 1.00 | 0.00 | 3A7 |
| ATOM | 1361 | CD1 | PHE | 213 | 28.391 | -8.264  | 10.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 1362 | CD2 | PHE | 213 | 29.890 | -9.399  | 9.039  | 1.00 | 0.00 | 3A7 |
| ATOM | 1363 | CE1 | PHE | 213 | 29.455 | -7.517  | 11.032 | 1.00 | 0.00 | 3A7 |
| ATOM | 1364 | CE2 | PHE | 213 | 30.959 | -8.666  | 9.546  | 1.00 | 0.00 | 3A7 |
| ATOM | 1365 | CZ  | PHE | 213 | 30.741 | -7.723  | 10.544 | 1.00 | 0.00 | 3A7 |
| ATOM | 1366 | C   | PHE | 213 | 27.926 | -12.408 | 9.426  | 1.00 | 0.00 | 3A7 |
| ATOM | 1367 | O   | PHE | 213 | 29.121 | -12.215 | 9.209  | 1.00 | 0.00 | 3A7 |
| ATOM | 1368 | N   | ASN | 214 | 27.395 | -13.649 | 9.491  | 1.00 | 0.00 | 3A7 |
| ATOM | 1369 | CA  | ASN | 214 | 28.142 | -14.839 | 9.165  | 1.00 | 0.00 | 3A7 |
| ATOM | 1370 | CB  | ASN | 214 | 29.054 | -15.372 | 10.314 | 1.00 | 0.00 | 3A7 |
| ATOM | 1371 | CG  | ASN | 214 | 29.994 | -16.484 | 9.818  | 1.00 | 0.00 | 3A7 |
| ATOM | 1372 | OD1 | ASN | 214 | 30.863 | -16.242 | 8.972  | 1.00 | 0.00 | 3A7 |
| ATOM | 1373 | ND2 | ASN | 214 | 29.800 | -17.720 | 10.370 | 1.00 | 0.00 | 3A7 |
| ATOM | 1374 | C   | ASN | 214 | 27.135 | -15.863 | 8.671  | 1.00 | 0.00 | 3A7 |
| ATOM | 1375 | O   | ASN | 214 | 27.356 | -16.351 | 7.565  | 1.00 | 0.00 | 3A7 |
| ATOM | 1376 | N   | PRO | 215 | 26.035 | -16.260 | 9.344  | 1.00 | 0.00 | 3A7 |
| ATOM | 1377 | CA  | PRO | 215 | 25.150 | -17.305 | 8.858  | 1.00 | 0.00 | 3A7 |
| ATOM | 1378 | CD  | PRO | 215 | 25.729 | -15.929 | 10.728 | 1.00 | 0.00 | 3A7 |
| ATOM | 1379 | CB  | PRO | 215 | 24.466 | -17.865 | 10.125 | 1.00 | 0.00 | 3A7 |
| ATOM | 1380 | CG  | PRO | 215 | 25.216 | -17.241 | 11.310 | 1.00 | 0.00 | 3A7 |
| ATOM | 1381 | C   | PRO | 215 | 24.158 | -16.681 | 7.893  | 1.00 | 0.00 | 3A7 |
| ATOM | 1382 | O   | PRO | 215 | 23.256 | -15.982 | 8.353  | 1.00 | 0.00 | 3A7 |
| ATOM | 1383 | N   | LEU | 216 | 24.323 | -16.921 | 6.560  | 1.00 | 0.00 | 3A7 |
| ATOM | 1384 | CA  | LEU | 216 | 23.496 | -16.424 | 5.463  | 1.00 | 0.00 | 3A7 |
| ATOM | 1385 | CB  | LEU | 216 | 21.971 | -16.737 | 5.575  | 1.00 | 0.00 | 3A7 |
| ATOM | 1386 | CG  | LEU | 216 | 21.559 | -18.224 | 5.393  | 1.00 | 0.00 | 3A7 |
| ATOM | 1387 | CD1 | LEU | 216 | 21.970 | -18.782 | 4.017  | 1.00 | 0.00 | 3A7 |
| ATOM | 1388 | CD2 | LEU | 216 | 22.012 | -19.148 | 6.540  | 1.00 | 0.00 | 3A7 |
| ATOM | 1389 | C   | LEU | 216 | 23.663 | -14.925 | 5.304  | 1.00 | 0.00 | 3A7 |
| ATOM | 1390 | O   | LEU | 216 | 22.996 | -14.143 | 5.980  | 1.00 | 0.00 | 3A7 |
| ATOM | 1391 | N   | ASP | 217 | 24.571 | -14.501 | 4.392  | 1.00 | 0.00 | 3A7 |
| ATOM | 1392 | CA  | ASP | 217 | 24.872 | -13.102 | 4.192  | 1.00 | 0.00 | 3A7 |
| ATOM | 1393 | CB  | ASP | 217 | 26.106 | -12.608 | 5.013  | 1.00 | 0.00 | 3A7 |
| ATOM | 1394 | CG  | ASP | 217 | 27.385 | -13.427 | 4.786  | 1.00 | 0.00 | 3A7 |
| ATOM | 1395 | OD1 | ASP | 217 | 28.378 | -12.833 | 4.285  | 1.00 | 0.00 | 3A7 |
| ATOM | 1396 | OD2 | ASP | 217 | 27.390 | -14.641 | 5.118  | 1.00 | 0.00 | 3A7 |



|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1397 | C   | ASP | 217 | 25.056 | -12.846 | 2.709  | 1.00 | 0.00 | 3A7 |
| ATOM | 1398 | O   | ASP | 217 | 26.126 | -13.118 | 2.166  | 1.00 | 0.00 | 3A7 |
| ATOM | 1399 | N   | PRO | 218 | 24.053 | -12.282 | 2.013  | 1.00 | 0.00 | 3A7 |
| ATOM | 1400 | CA  | PRO | 218 | 24.193 | -11.689 | 0.691  | 1.00 | 0.00 | 3A7 |
| ATOM | 1401 | CD  | PRO | 218 | 22.655 | -12.450 | 2.382  | 1.00 | 0.00 | 3A7 |
| ATOM | 1402 | CB  | PRO | 218 | 22.746 | -11.477 | 0.203  | 1.00 | 0.00 | 3A7 |
| ATOM | 1403 | CG  | PRO | 218 | 21.908 | -12.439 | 1.050  | 1.00 | 0.00 | 3A7 |
| ATOM | 1404 | C   | PRO | 218 | 24.945 | -10.372 | 0.782  | 1.00 | 0.00 | 3A7 |
| ATOM | 1405 | O   | PRO | 218 | 24.911 | -9.730  | 1.833  | 1.00 | 0.00 | 3A7 |
| ATOM | 1406 | N   | PHE | 219 | 25.621 | -9.950  | -0.316 | 1.00 | 0.00 | 3A7 |
| ATOM | 1407 | CA  | PHE | 219 | 26.432 | -8.745  | -0.344 | 1.00 | 0.00 | 3A7 |
| ATOM | 1408 | CB  | PHE | 219 | 27.591 | -8.800  | -1.373 | 1.00 | 0.00 | 3A7 |
| ATOM | 1409 | CG  | PHE | 219 | 28.495 | -9.952  | -1.047 | 1.00 | 0.00 | 3A7 |
| ATOM | 1410 | CD1 | PHE | 219 | 29.296 | -9.917  | 0.094  | 1.00 | 0.00 | 3A7 |
| ATOM | 1411 | CD2 | PHE | 219 | 28.551 | -11.070 | -1.881 | 1.00 | 0.00 | 3A7 |
| ATOM | 1412 | CE1 | PHE | 219 | 30.140 | -10.981 | 0.400  | 1.00 | 0.00 | 3A7 |
| ATOM | 1413 | CE2 | PHE | 219 | 29.393 | -12.136 | -1.578 | 1.00 | 0.00 | 3A7 |
| ATOM | 1414 | CZ  | PHE | 219 | 30.189 | -12.092 | -0.437 | 1.00 | 0.00 | 3A7 |
| ATOM | 1415 | C   | PHE | 219 | 25.587 | -7.501  | -0.570 | 1.00 | 0.00 | 3A7 |
| ATOM | 1416 | O   | PHE | 219 | 25.626 | -6.607  | 0.273  | 1.00 | 0.00 | 3A7 |
| ATOM | 1417 | N   | VAL | 220 | 24.790 | -7.366  | -1.669 | 1.00 | 0.00 | 3A7 |
| ATOM | 1418 | CA  | VAL | 220 | 24.617 | -8.245  | -2.807 | 1.00 | 0.00 | 3A7 |
| ATOM | 1419 | CB  | VAL | 220 | 23.148 | -8.591  | -3.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 1420 | CG1 | VAL | 220 | 22.271 | -7.323  | -3.127 | 1.00 | 0.00 | 3A7 |
| ATOM | 1421 | CG2 | VAL | 220 | 22.991 | -9.517  | -4.277 | 1.00 | 0.00 | 3A7 |
| ATOM | 1422 | C   | VAL | 220 | 25.287 | -7.570  | -3.983 | 1.00 | 0.00 | 3A7 |
| ATOM | 1423 | O   | VAL | 220 | 25.799 | -8.235  | -4.883 | 1.00 | 0.00 | 3A7 |
| ATOM | 1424 | N   | LEU | 221 | 25.336 | -6.211  | -3.963 | 1.00 | 0.00 | 3A7 |
| ATOM | 1425 | CA  | LEU | 221 | 26.163 | -5.403  | -4.835 | 1.00 | 0.00 | 3A7 |
| ATOM | 1426 | CB  | LEU | 221 | 25.390 | -4.284  | -5.597 | 1.00 | 0.00 | 3A7 |
| ATOM | 1427 | CG  | LEU | 221 | 24.479 | -4.750  | -6.764 | 1.00 | 0.00 | 3A7 |
| ATOM | 1428 | CD1 | LEU | 221 | 25.258 | -5.539  | -7.835 | 1.00 | 0.00 | 3A7 |
| ATOM | 1429 | CD2 | LEU | 221 | 23.213 | -5.501  | -6.317 | 1.00 | 0.00 | 3A7 |
| ATOM | 1430 | C   | LEU | 221 | 27.196 | -4.792  | -3.913 | 1.00 | 0.00 | 3A7 |
| ATOM | 1431 | O   | LEU | 221 | 27.565 | -5.391  | -2.904 | 1.00 | 0.00 | 3A7 |
| ATOM | 1432 | N   | SER | 222 | 27.682 | -3.567  | -4.239 | 1.00 | 0.00 | 3A7 |
| ATOM | 1433 | CA  | SER | 222 | 28.622 | -2.816  | -3.435 | 1.00 | 0.00 | 3A7 |
| ATOM | 1434 | CB  | SER | 222 | 29.722 | -2.139  | -4.284 | 1.00 | 0.00 | 3A7 |
| ATOM | 1435 | OG  | SER | 222 | 30.472 | -3.121  | -4.985 | 1.00 | 0.00 | 3A7 |
| ATOM | 1436 | C   | SER | 222 | 27.841 | -1.762  | -2.698 | 1.00 | 0.00 | 3A7 |
| ATOM | 1437 | O   | SER | 222 | 27.764 | -0.612  | -3.127 | 1.00 | 0.00 | 3A7 |
| ATOM | 1438 | N   | ILE | 223 | 27.222 | -2.164  | -1.561 | 1.00 | 0.00 | 3A7 |
| ATOM | 1439 | CA  | ILE | 223 | 26.322 | -1.338  | -0.788 | 1.00 | 0.00 | 3A7 |
| ATOM | 1440 | CB  | ILE | 223 | 24.971 | -2.017  | -0.555 | 1.00 | 0.00 | 3A7 |
| ATOM | 1441 | CG2 | ILE | 223 | 25.156 | -3.487  | -0.110 | 1.00 | 0.00 | 3A7 |
| ATOM | 1442 | CG1 | ILE | 223 | 24.042 | -1.193  | 0.374  | 1.00 | 0.00 | 3A7 |
| ATOM | 1443 | CD  | ILE | 223 | 22.603 | -1.718  | 0.416  | 1.00 | 0.00 | 3A7 |
| ATOM | 1444 | C   | ILE | 223 | 27.019 | -0.926  | 0.488  | 1.00 | 0.00 | 3A7 |
| ATOM | 1445 | O   | ILE | 223 | 27.093 | 0.266   | 0.787  | 1.00 | 0.00 | 3A7 |
| ATOM | 1446 | N   | LYS | 224 | 27.556 | -1.893  | 1.271  | 1.00 | 0.00 | 3A7 |
| ATOM | 1447 | CA  | LYS | 224 | 28.263 | -1.581  | 2.490  | 1.00 | 0.00 | 3A7 |
| ATOM | 1448 | CB  | LYS | 224 | 27.339 | -1.185  | 3.674  | 1.00 | 0.00 | 3A7 |
| ATOM | 1449 | CG  | LYS | 224 | 28.088 | -0.528  | 4.849  | 1.00 | 0.00 | 3A7 |
| ATOM | 1450 | CD  | LYS | 224 | 27.190 | -0.187  | 6.049  | 1.00 | 0.00 | 3A7 |
| ATOM | 1451 | CE  | LYS | 224 | 26.740 | -1.411  | 6.861  | 1.00 | 0.00 | 3A7 |
| ATOM | 1452 | NZ  | LYS | 224 | 27.901 | -2.112  | 7.458  | 1.00 | 0.00 | 3A7 |
| ATOM | 1453 | C   | LYS | 224 | 29.052 | -2.796  | 2.890  | 1.00 | 0.00 | 3A7 |
| ATOM | 1454 | O   | LYS | 224 | 30.070 | -2.683  | 3.572  | 1.00 | 0.00 | 3A7 |
| ATOM | 1455 | N   | VAL | 225 | 28.582 | -4.008  | 2.483  | 1.00 | 0.00 | 3A7 |
| ATOM | 1456 | CA  | VAL | 225 | 29.124 | -5.288  | 2.907  | 1.00 | 0.00 | 3A7 |
| ATOM | 1457 | CB  | VAL | 225 | 28.125 | -6.430  | 2.746  | 1.00 | 0.00 | 3A7 |
| ATOM | 1458 | CG1 | VAL | 225 | 28.683 | -7.731  | 3.365  | 1.00 | 0.00 | 3A7 |
| ATOM | 1459 | CG2 | VAL | 225 | 26.805 | -6.017  | 3.429  | 1.00 | 0.00 | 3A7 |
| ATOM | 1460 | C   | VAL | 225 | 30.398 | -5.583  | 2.147  | 1.00 | 0.00 | 3A7 |
| ATOM | 1461 | O   | VAL | 225 | 31.486 | -5.449  | 2.708  | 1.00 | 0.00 | 3A7 |
| ATOM | 1462 | N   | PHE | 226 | 30.271 | -5.986  | 0.851  | 1.00 | 0.00 | 3A7 |
| ATOM | 1463 | CA  | PHE | 226 | 31.349 | -6.182  | -0.106 | 1.00 | 0.00 | 3A7 |
| ATOM | 1464 | CB  | PHE | 226 | 32.367 | -4.997  | -0.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 1465 | CG  | PHE | 226 | 33.203 | -4.921  | -1.346 | 1.00 | 0.00 | 3A7 |
| ATOM | 1466 | CD1 | PHE | 226 | 34.585 | -5.107  | -1.283 | 1.00 | 0.00 | 3A7 |
| ATOM | 1467 | CD2 | PHE | 226 | 32.615 | -4.631  | -2.578 | 1.00 | 0.00 | 3A7 |
| ATOM | 1468 | CE1 | PHE | 226 | 35.365 | -5.025  | -2.432 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1469 | CE2 | PHE | 226 | 33.393 | -4.550  | -3.730 | 1.00 | 0.00 | 3A7 |
| ATOM | 1470 | CZ  | PHE | 226 | 34.768 | -4.749  | -3.658 | 1.00 | 0.00 | 3A7 |
| ATOM | 1471 | C   | PHE | 226 | 32.059 | -7.514  | 0.144  | 1.00 | 0.00 | 3A7 |
| ATOM | 1472 | O   | PHE | 226 | 32.151 | -7.943  | 1.295  | 1.00 | 0.00 | 3A7 |
| ATOM | 1473 | N   | PRO | 227 | 32.610 | -8.198  | -0.871 | 1.00 | 0.00 | 3A7 |
| ATOM | 1474 | CA  | PRO | 227 | 33.431 | -9.392  | -0.698 | 1.00 | 0.00 | 3A7 |
| ATOM | 1475 | CD  | PRO | 227 | 32.111 | -8.089  | -2.237 | 1.00 | 0.00 | 3A7 |
| ATOM | 1476 | CB  | PRO | 227 | 33.602 | -9.944  | -2.123 | 1.00 | 0.00 | 3A7 |
| ATOM | 1477 | CG  | PRO | 227 | 32.349 | -9.465  | -2.857 | 1.00 | 0.00 | 3A7 |
| ATOM | 1478 | C   | PRO | 227 | 34.778 | -9.081  | -0.061 | 1.00 | 0.00 | 3A7 |
| ATOM | 1479 | O   | PRO | 227 | 35.140 | -7.911  | 0.062  | 1.00 | 0.00 | 3A7 |
| ATOM | 1480 | N   | PHE | 228 | 35.535 | -10.132 | 0.346  | 1.00 | 0.00 | 3A7 |
| ATOM | 1481 | CA  | PHE | 228 | 36.792 | -10.004 | 1.060  | 1.00 | 0.00 | 3A7 |
| ATOM | 1482 | CB  | PHE | 228 | 37.130 | -11.255 | 1.926  | 1.00 | 0.00 | 3A7 |
| ATOM | 1483 | CG  | PHE | 228 | 37.053 | -12.560 | 1.172  | 1.00 | 0.00 | 3A7 |
| ATOM | 1484 | CD1 | PHE | 228 | 35.821 | -13.176 | 0.937  | 1.00 | 0.00 | 3A7 |
| ATOM | 1485 | CD2 | PHE | 228 | 38.217 | -13.193 | 0.733  | 1.00 | 0.00 | 3A7 |
| ATOM | 1486 | CE1 | PHE | 228 | 35.753 | -14.388 | 0.257  | 1.00 | 0.00 | 3A7 |
| ATOM | 1487 | CE2 | PHE | 228 | 38.152 | -14.405 | 0.053  | 1.00 | 0.00 | 3A7 |
| ATOM | 1488 | CZ  | PHE | 228 | 36.919 | -15.003 | -0.187 | 1.00 | 0.00 | 3A7 |
| ATOM | 1489 | C   | PHE | 228 | 37.924 | -9.676  | 0.107  | 1.00 | 0.00 | 3A7 |
| ATOM | 1490 | O   | PHE | 228 | 38.323 | -10.488 | -0.727 | 1.00 | 0.00 | 3A7 |
| ATOM | 1491 | N   | LEU | 229 | 38.440 | -8.432  | 0.225  | 1.00 | 0.00 | 3A7 |
| ATOM | 1492 | CA  | LEU | 229 | 39.469 | -7.914  | -0.636 | 1.00 | 0.00 | 3A7 |
| ATOM | 1493 | CB  | LEU | 229 | 38.924 | -7.440  | -2.010 | 1.00 | 0.00 | 3A7 |
| ATOM | 1494 | CG  | LEU | 229 | 39.979 | -6.871  | -2.990 | 1.00 | 0.00 | 3A7 |
| ATOM | 1495 | CD1 | LEU | 229 | 41.083 | -7.892  | -3.326 | 1.00 | 0.00 | 3A7 |
| ATOM | 1496 | CD2 | LEU | 229 | 39.305 | -6.347  | -4.273 | 1.00 | 0.00 | 3A7 |
| ATOM | 1497 | C   | LEU | 229 | 40.062 | -6.752  | 0.105  | 1.00 | 0.00 | 3A7 |
| ATOM | 1498 | O   | LEU | 229 | 41.281 | -6.639  | 0.226  | 1.00 | 0.00 | 3A7 |
| ATOM | 1499 | N   | THR | 230 | 39.186 | -5.847  | 0.615  | 1.00 | 0.00 | 3A7 |
| ATOM | 1500 | CA  | THR | 230 | 39.568 | -4.636  | 1.308  | 1.00 | 0.00 | 3A7 |
| ATOM | 1501 | CB  | THR | 230 | 38.715 | -3.444  | 0.870  | 1.00 | 0.00 | 3A7 |
| ATOM | 1502 | OG1 | THR | 230 | 39.184 | -2.215  | 1.417  | 1.00 | 0.00 | 3A7 |
| ATOM | 1503 | CG2 | THR | 230 | 37.220 | -3.639  | 1.206  | 1.00 | 0.00 | 3A7 |
| ATOM | 1504 | C   | THR | 230 | 39.476 | -4.902  | 2.807  | 1.00 | 0.00 | 3A7 |
| ATOM | 1505 | O   | THR | 230 | 38.513 | -5.527  | 3.250  | 1.00 | 0.00 | 3A7 |
| ATOM | 1506 | N   | PRO | 231 | 40.435 | -4.450  | 3.626  | 1.00 | 0.00 | 3A7 |
| ATOM | 1507 | CA  | PRO | 231 | 40.382 | -4.534  | 5.074  | 1.00 | 0.00 | 3A7 |
| ATOM | 1508 | CD  | PRO | 231 | 41.737 | -3.996  | 3.151  | 1.00 | 0.00 | 3A7 |
| ATOM | 1509 | CB  | PRO | 231 | 41.866 | -4.556  | 5.472  | 1.00 | 0.00 | 3A7 |
| ATOM | 1510 | CG  | PRO | 231 | 42.555 | -3.696  | 4.409  | 1.00 | 0.00 | 3A7 |
| ATOM | 1511 | C   | PRO | 231 | 39.661 | -3.313  | 5.625  | 1.00 | 0.00 | 3A7 |
| ATOM | 1512 | O   | PRO | 231 | 38.946 | -2.637  | 4.885  | 1.00 | 0.00 | 3A7 |
| ATOM | 1513 | N   | ILE | 232 | 39.877 | -3.024  | 6.939  | 1.00 | 0.00 | 3A7 |
| ATOM | 1514 | CA  | ILE | 232 | 39.462 | -1.870  | 7.738  | 1.00 | 0.00 | 3A7 |
| ATOM | 1515 | CB  | ILE | 232 | 40.410 | -0.663  | 7.563  | 1.00 | 0.00 | 3A7 |
| ATOM | 1516 | CG2 | ILE | 232 | 40.450 | -0.093  | 6.123  | 1.00 | 0.00 | 3A7 |
| ATOM | 1517 | CG1 | ILE | 232 | 40.186 | 0.463   | 8.608  | 1.00 | 0.00 | 3A7 |
| ATOM | 1518 | CD  | ILE | 232 | 40.563 | 0.068   | 10.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 1519 | C   | ILE | 232 | 37.983 | -1.493  | 7.610  | 1.00 | 0.00 | 3A7 |
| ATOM | 1520 | O   | ILE | 232 | 37.631 | -0.517  | 6.949  | 1.00 | 0.00 | 3A7 |
| ATOM | 1521 | N   | LEU | 233 | 37.047 | -2.244  | 8.259  | 1.00 | 0.00 | 3A7 |
| ATOM | 1522 | CA  | LEU | 233 | 37.231 | -3.488  | 8.977  | 1.00 | 0.00 | 3A7 |
| ATOM | 1523 | CB  | LEU | 233 | 36.638 | -3.490  | 10.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 1524 | CG  | LEU | 233 | 37.361 | -2.613  | 11.475 | 1.00 | 0.00 | 3A7 |
| ATOM | 1525 | CD1 | LEU | 233 | 38.832 | -3.029  | 11.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 1526 | CD2 | LEU | 233 | 37.198 | -1.098  | 11.249 | 1.00 | 0.00 | 3A7 |
| ATOM | 1527 | C   | LEU | 233 | 36.518 | -4.523  | 8.138  | 1.00 | 0.00 | 3A7 |
| ATOM | 1528 | O   | LEU | 233 | 36.754 | -4.608  | 6.933  | 1.00 | 0.00 | 3A7 |
| ATOM | 1529 | N   | GLU | 234 | 35.621 | -5.330  | 8.775  | 1.00 | 0.00 | 3A7 |
| ATOM | 1530 | CA  | GLU | 234 | 34.755 | -6.337  | 8.183  | 1.00 | 0.00 | 3A7 |
| ATOM | 1531 | CB  | GLU | 234 | 33.985 | -5.836  | 6.925  | 1.00 | 0.00 | 3A7 |
| ATOM | 1532 | CG  | GLU | 234 | 32.750 | -6.666  | 6.514  | 1.00 | 0.00 | 3A7 |
| ATOM | 1533 | CD  | GLU | 234 | 33.141 | -7.946  | 5.777  | 1.00 | 0.00 | 3A7 |
| ATOM | 1534 | OE1 | GLU | 234 | 33.797 | -7.837  | 4.707  | 1.00 | 0.00 | 3A7 |
| ATOM | 1535 | OE2 | GLU | 234 | 32.780 | -9.048  | 6.271  | 1.00 | 0.00 | 3A7 |
| ATOM | 1536 | C   | GLU | 234 | 35.545 | -7.587  | 7.877  | 1.00 | 0.00 | 3A7 |
| ATOM | 1537 | O   | GLU | 234 | 36.385 | -7.576  | 6.978  | 1.00 | 0.00 | 3A7 |
| ATOM | 1538 | N   | ALA | 235 | 35.267 | -8.681  | 8.642  | 1.00 | 0.00 | 3A7 |
| ATOM | 1539 | CA  | ALA | 235 | 35.833 | -10.014 | 8.499  | 1.00 | 0.00 | 3A7 |
| ATOM | 1540 | CB  | ALA | 235 | 36.269 | -10.390 | 7.067  | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1541 | C   | ALA | 235 | 37.017 | -10.214 | 9.409  | 1.00 | 0.00 | 3A7 |
| ATOM | 1542 | O   | ALA | 235 | 37.273 | -11.312 | 9.899  | 1.00 | 0.00 | 3A7 |
| ATOM | 1543 | N   | LEU | 236 | 37.790 | -9.141  | 9.671  | 1.00 | 0.00 | 3A7 |
| ATOM | 1544 | CA  | LEU | 236 | 38.971 | -9.206  | 10.503 | 1.00 | 0.00 | 3A7 |
| ATOM | 1545 | CB  | LEU | 236 | 39.828 | -7.935  | 10.361 | 1.00 | 0.00 | 3A7 |
| ATOM | 1546 | CG  | LEU | 236 | 40.242 | -7.612  | 8.906  | 1.00 | 0.00 | 3A7 |
| ATOM | 1547 | CD1 | LEU | 236 | 40.964 | -6.254  | 8.836  | 1.00 | 0.00 | 3A7 |
| ATOM | 1548 | CD2 | LEU | 236 | 41.094 | -8.728  | 8.272  | 1.00 | 0.00 | 3A7 |
| ATOM | 1549 | C   | LEU | 236 | 38.601 | -9.366  | 11.956 | 1.00 | 0.00 | 3A7 |
| ATOM | 1550 | O   | LEU | 236 | 39.204 | -10.138 | 12.697 | 1.00 | 0.00 | 3A7 |
| ATOM | 1551 | N   | ASN | 237 | 37.530 | -8.664  | 12.387 | 1.00 | 0.00 | 3A7 |
| ATOM | 1552 | CA  | ASN | 237 | 37.020 | -8.738  | 13.741 | 1.00 | 0.00 | 3A7 |
| ATOM | 1553 | CB  | ASN | 237 | 35.917 | -7.685  | 13.982 | 1.00 | 0.00 | 3A7 |
| ATOM | 1554 | CG  | ASN | 237 | 36.463 | -6.273  | 13.746 | 1.00 | 0.00 | 3A7 |
| ATOM | 1555 | OD1 | ASN | 237 | 35.922 | -5.526  | 12.923 | 1.00 | 0.00 | 3A7 |
| ATOM | 1556 | ND2 | ASN | 237 | 37.544 | -5.910  | 14.500 | 1.00 | 0.00 | 3A7 |
| ATOM | 1557 | C   | ASN | 237 | 36.444 | -10.107 | 14.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 1558 | O   | ASN | 237 | 36.569 | -10.658 | 15.111 | 1.00 | 0.00 | 3A7 |
| ATOM | 1559 | N   | ILE | 238 | 35.832 | -10.707 | 12.979 | 1.00 | 0.00 | 3A7 |
| ATOM | 1560 | CA  | ILE | 238 | 35.229 | -12.011 | 13.021 | 1.00 | 0.00 | 3A7 |
| ATOM | 1561 | CB  | ILE | 238 | 34.447 | -12.290 | 11.743 | 1.00 | 0.00 | 3A7 |
| ATOM | 1562 | CG2 | ILE | 238 | 33.714 | -13.648 | 11.845 | 1.00 | 0.00 | 3A7 |
| ATOM | 1563 | CG1 | ILE | 238 | 33.451 | -11.141 | 11.432 | 1.00 | 0.00 | 3A7 |
| ATOM | 1564 | CD  | ILE | 238 | 32.367 | -10.932 | 12.495 | 1.00 | 0.00 | 3A7 |
| ATOM | 1565 | C   | ILE | 238 | 36.280 | -13.064 | 13.260 | 1.00 | 0.00 | 3A7 |
| ATOM | 1566 | O   | ILE | 238 | 36.094 | -13.896 | 14.106 | 1.00 | 0.00 | 3A7 |
| ATOM | 1567 | N   | THR | 239 | 37.422 | -13.013 | 12.556 | 1.00 | 0.00 | 3A7 |
| ATOM | 1568 | CA  | THR | 239 | 38.535 | -13.929 | 12.699 | 1.00 | 0.00 | 3A7 |
| ATOM | 1569 | CB  | THR | 239 | 39.546 | -13.767 | 11.574 | 1.00 | 0.00 | 3A7 |
| ATOM | 1570 | OG1 | THR | 239 | 38.870 | -13.766 | 10.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 1571 | CG2 | THR | 239 | 40.562 | -14.928 | 11.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 1572 | C   | THR | 239 | 39.226 | -13.773 | 14.033 | 1.00 | 0.00 | 3A7 |
| ATOM | 1573 | O   | THR | 239 | 39.720 | -14.740 | 14.603 | 1.00 | 0.00 | 3A7 |
| ATOM | 1574 | N   | VAL | 240 | 39.204 | -12.555 | 14.619 | 1.00 | 0.00 | 3A7 |
| ATOM | 1575 | CA  | VAL | 240 | 39.759 | -12.276 | 15.932 | 1.00 | 0.00 | 3A7 |
| ATOM | 1576 | CB  | VAL | 240 | 39.930 | -10.784 | 16.162 | 1.00 | 0.00 | 3A7 |
| ATOM | 1577 | CG1 | VAL | 240 | 40.276 | -10.421 | 17.627 | 1.00 | 0.00 | 3A7 |
| ATOM | 1578 | CG2 | VAL | 240 | 41.076 | -10.316 | 15.239 | 1.00 | 0.00 | 3A7 |
| ATOM | 1579 | C   | VAL | 240 | 38.911 | -12.842 | 17.025 | 1.00 | 0.00 | 3A7 |
| ATOM | 1580 | O   | VAL | 240 | 39.418 | -13.460 | 17.956 | 1.00 | 0.00 | 3A7 |
| ATOM | 1581 | N   | PHE | 241 | 37.578 | -12.667 | 16.920 | 1.00 | 0.00 | 3A7 |
| ATOM | 1582 | CA  | PHE | 241 | 36.634 | -13.266 | 17.837 | 1.00 | 0.00 | 3A7 |
| ATOM | 1583 | CB  | PHE | 241 | 35.170 | -12.893 | 17.483 | 1.00 | 0.00 | 3A7 |
| ATOM | 1584 | CG  | PHE | 241 | 34.222 | -14.041 | 17.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 1585 | CD1 | PHE | 241 | 33.928 | -15.104 | 17.973 | 1.00 | 0.00 | 3A7 |
| ATOM | 1586 | CD2 | PHE | 241 | 34.038 | -14.250 | 15.746 | 1.00 | 0.00 | 3A7 |
| ATOM | 1587 | CE1 | PHE | 241 | 33.801 | -16.400 | 17.483 | 1.00 | 0.00 | 3A7 |
| ATOM | 1588 | CE2 | PHE | 241 | 34.006 | -15.545 | 15.244 | 1.00 | 0.00 | 3A7 |
| ATOM | 1589 | CZ  | PHE | 241 | 33.918 | -16.626 | 16.119 | 1.00 | 0.00 | 3A7 |
| ATOM | 1590 | C   | PHE | 241 | 36.784 | -14.763 | 17.938 | 1.00 | 0.00 | 3A7 |
| ATOM | 1591 | O   | PHE | 241 | 36.807 | -15.276 | 19.050 | 1.00 | 0.00 | 3A7 |
| ATOM | 1592 | N   | PRO | 242 | 36.833 | -15.511 | 16.814 | 1.00 | 0.00 | 3A7 |
| ATOM | 1593 | CA  | PRO | 242 | 36.972 | -16.902 | 16.784 | 1.00 | 0.00 | 3A7 |
| ATOM | 1594 | CD  | PRO | 242 | 37.457 | -15.196 | 15.686 | 1.00 | 0.00 | 3A7 |
| ATOM | 1595 | CB  | PRO | 242 | 36.945 | -17.375 | 15.333 | 1.00 | 0.00 | 3A7 |
| ATOM | 1596 | CG  | PRO | 242 | 37.313 | -16.221 | 14.553 | 1.00 | 0.00 | 3A7 |
| ATOM | 1597 | C   | PRO | 242 | 38.274 | -17.310 | 17.435 | 1.00 | 0.00 | 3A7 |
| ATOM | 1598 | O   | PRO | 242 | 38.251 | -18.268 | 18.191 | 1.00 | 0.00 | 3A7 |
| ATOM | 1599 | N   | ARG | 243 | 39.409 | -16.603 | 17.262 | 1.00 | 0.00 | 3A7 |
| ATOM | 1600 | CA  | ARG | 243 | 40.651 | -16.892 | 17.893 | 1.00 | 0.00 | 3A7 |
| ATOM | 1601 | CB  | ARG | 243 | 41.734 | -15.942 | 17.355 | 1.00 | 0.00 | 3A7 |
| ATOM | 1602 | CG  | ARG | 243 | 42.172 | -16.265 | 15.917 | 1.00 | 0.00 | 3A7 |
| ATOM | 1603 | CD  | ARG | 243 | 43.102 | -15.187 | 15.348 | 1.00 | 0.00 | 3A7 |
| ATOM | 1604 | NE  | ARG | 243 | 43.425 | -15.532 | 13.927 | 1.00 | 0.00 | 3A7 |
| ATOM | 1605 | CZ  | ARG | 243 | 44.062 | -14.651 | 13.096 | 1.00 | 0.00 | 3A7 |
| ATOM | 1606 | NH1 | ARG | 243 | 44.310 | -15.003 | 11.800 | 1.00 | 0.00 | 3A7 |
| ATOM | 1607 | NH2 | ARG | 243 | 44.444 | -13.422 | 13.549 | 1.00 | 0.00 | 3A7 |
| ATOM | 1608 | C   | ARG | 243 | 40.582 | -16.769 | 19.398 | 1.00 | 0.00 | 3A7 |
| ATOM | 1609 | O   | ARG | 243 | 41.152 | -17.580 | 20.122 | 1.00 | 0.00 | 3A7 |
| ATOM | 1610 | N   | LYS | 244 | 39.813 | -15.774 | 19.905 | 1.00 | 0.00 | 3A7 |
| ATOM | 1611 | CA  | LYS | 244 | 39.642 | -15.565 | 21.327 | 1.00 | 0.00 | 3A7 |
| ATOM | 1612 | CB  | LYS | 244 | 39.046 | -14.178 | 21.648 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1613 | CG  | LYS | 244 | 39.241 | -13.772 | 23.119 | 1.00 | 0.00 | 3A7 |
| ATOM | 1614 | CD  | LYS | 244 | 39.058 | -12.271 | 23.402 | 1.00 | 0.00 | 3A7 |
| ATOM | 1615 | CE  | LYS | 244 | 40.110 | -11.365 | 22.745 | 1.00 | 0.00 | 3A7 |
| ATOM | 1616 | NZ  | LYS | 244 | 41.474 | -11.713 | 23.205 | 1.00 | 0.00 | 3A7 |
| ATOM | 1617 | C   | LYS | 244 | 38.844 | -16.684 | 21.965 | 1.00 | 0.00 | 3A7 |
| ATOM | 1618 | O   | LYS | 244 | 39.175 | -17.150 | 23.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 1619 | N   | VAL | 245 | 37.806 | -17.201 | 21.259 | 1.00 | 0.00 | 3A7 |
| ATOM | 1620 | CA  | VAL | 245 | 37.014 | -18.341 | 21.692 | 1.00 | 0.00 | 3A7 |
| ATOM | 1621 | CB  | VAL | 245 | 35.821 | -18.595 | 20.774 | 1.00 | 0.00 | 3A7 |
| ATOM | 1622 | CG1 | VAL | 245 | 35.055 | -19.885 | 21.138 | 1.00 | 0.00 | 3A7 |
| ATOM | 1623 | CG2 | VAL | 245 | 34.893 | -17.368 | 20.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 1624 | C   | VAL | 245 | 37.868 | -19.581 | 21.753 | 1.00 | 0.00 | 3A7 |
| ATOM | 1625 | O   | VAL | 245 | 37.867 | -20.306 | 22.748 | 1.00 | 0.00 | 3A7 |
| ATOM | 1626 | N   | ILE | 246 | 38.674 | -19.822 | 20.690 | 1.00 | 0.00 | 3A7 |
| ATOM | 1627 | CA  | ILE | 246 | 39.563 | -20.965 | 20.600 | 1.00 | 0.00 | 3A7 |
| ATOM | 1628 | CB  | ILE | 246 | 40.252 | -21.026 | 19.232 | 1.00 | 0.00 | 3A7 |
| ATOM | 1629 | CG2 | ILE | 246 | 41.696 | -21.593 | 19.259 | 1.00 | 0.00 | 3A7 |
| ATOM | 1630 | CG1 | ILE | 246 | 39.414 | -21.855 | 18.224 | 1.00 | 0.00 | 3A7 |
| ATOM | 1631 | CD  | ILE | 246 | 38.083 | -21.241 | 17.793 | 1.00 | 0.00 | 3A7 |
| ATOM | 1632 | C   | ILE | 246 | 40.571 | -20.966 | 21.724 | 1.00 | 0.00 | 3A7 |
| ATOM | 1633 | O   | ILE | 246 | 40.828 | -21.996 | 22.332 | 1.00 | 0.00 | 3A7 |
| ATOM | 1634 | N   | SER | 247 | 41.133 | -19.787 | 22.059 | 1.00 | 0.00 | 3A7 |
| ATOM | 1635 | CA  | SER | 247 | 42.119 | -19.652 | 23.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 1636 | CB  | SER | 247 | 42.734 | -18.250 | 23.119 | 1.00 | 0.00 | 3A7 |
| ATOM | 1637 | OG  | SER | 247 | 43.425 | -18.000 | 21.903 | 1.00 | 0.00 | 3A7 |
| ATOM | 1638 | C   | SER | 247 | 41.551 | -19.917 | 24.461 | 1.00 | 0.00 | 3A7 |
| ATOM | 1639 | O   | SER | 247 | 42.194 | -20.579 | 25.271 | 1.00 | 0.00 | 3A7 |
| ATOM | 1640 | N   | PHE | 248 | 40.320 | -19.434 | 24.749 | 1.00 | 0.00 | 3A7 |
| ATOM | 1641 | CA  | PHE | 248 | 39.670 | -19.654 | 26.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 1642 | CB  | PHE | 248 | 38.328 | -18.900 | 26.125 | 1.00 | 0.00 | 3A7 |
| ATOM | 1643 | CG  | PHE | 248 | 38.514 | -17.473 | 26.559 | 1.00 | 0.00 | 3A7 |
| ATOM | 1644 | CD1 | PHE | 248 | 37.951 | -16.425 | 25.828 | 1.00 | 0.00 | 3A7 |
| ATOM | 1645 | CD2 | PHE | 248 | 39.191 | -17.176 | 27.745 | 1.00 | 0.00 | 3A7 |
| ATOM | 1646 | CE1 | PHE | 248 | 38.058 | -15.111 | 26.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 1647 | CE2 | PHE | 248 | 39.316 | -15.861 | 28.183 | 1.00 | 0.00 | 3A7 |
| ATOM | 1648 | CZ  | PHE | 248 | 38.749 | -14.827 | 27.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 1649 | C   | PHE | 248 | 39.389 | -21.122 | 26.244 | 1.00 | 0.00 | 3A7 |
| ATOM | 1650 | O   | PHE | 248 | 39.623 | -21.663 | 27.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 1651 | N   | LEU | 249 | 38.919 | -21.832 | 25.198 | 1.00 | 0.00 | 3A7 |
| ATOM | 1652 | CA  | LEU | 249 | 38.585 | -23.234 | 25.317 | 1.00 | 0.00 | 3A7 |
| ATOM | 1653 | CB  | LEU | 249 | 37.717 | -23.699 | 24.147 | 1.00 | 0.00 | 3A7 |
| ATOM | 1654 | CG  | LEU | 249 | 36.376 | -22.962 | 24.103 | 1.00 | 0.00 | 3A7 |
| ATOM | 1655 | CD1 | LEU | 249 | 35.616 | -23.308 | 22.821 | 1.00 | 0.00 | 3A7 |
| ATOM | 1656 | CD2 | LEU | 249 | 35.503 | -23.243 | 25.342 | 1.00 | 0.00 | 3A7 |
| ATOM | 1657 | C   | LEU | 249 | 39.811 | -24.111 | 25.396 | 1.00 | 0.00 | 3A7 |
| ATOM | 1658 | O   | LEU | 249 | 39.841 | -25.088 | 26.140 | 1.00 | 0.00 | 3A7 |
| ATOM | 1659 | N   | THR | 250 | 40.891 | -23.744 | 24.670 | 1.00 | 0.00 | 3A7 |
| ATOM | 1660 | CA  | THR | 250 | 42.150 | -24.464 | 24.706 | 1.00 | 0.00 | 3A7 |
| ATOM | 1661 | CB  | THR | 250 | 43.131 | -23.926 | 23.673 | 1.00 | 0.00 | 3A7 |
| ATOM | 1662 | OG1 | THR | 250 | 42.595 | -24.120 | 22.372 | 1.00 | 0.00 | 3A7 |
| ATOM | 1663 | CG2 | THR | 250 | 44.496 | -24.649 | 23.731 | 1.00 | 0.00 | 3A7 |
| ATOM | 1664 | C   | THR | 250 | 42.765 | -24.398 | 26.085 | 1.00 | 0.00 | 3A7 |
| ATOM | 1665 | O   | THR | 250 | 43.326 | -25.376 | 26.573 | 1.00 | 0.00 | 3A7 |
| ATOM | 1666 | N   | LYS | 251 | 42.622 | -23.243 | 26.777 | 1.00 | 0.00 | 3A7 |
| ATOM | 1667 | CA  | LYS | 251 | 43.087 | -23.060 | 28.132 | 1.00 | 0.00 | 3A7 |
| ATOM | 1668 | CB  | LYS | 251 | 42.941 | -21.601 | 28.592 | 1.00 | 0.00 | 3A7 |
| ATOM | 1669 | CG  | LYS | 251 | 43.599 | -21.282 | 29.945 | 1.00 | 0.00 | 3A7 |
| ATOM | 1670 | CD  | LYS | 251 | 43.466 | -19.803 | 30.335 | 1.00 | 0.00 | 3A7 |
| ATOM | 1671 | CE  | LYS | 251 | 44.093 | -19.494 | 31.700 | 1.00 | 0.00 | 3A7 |
| ATOM | 1672 | NZ  | LYS | 251 | 43.930 | -18.062 | 32.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 1673 | C   | LYS | 251 | 42.337 | -23.933 | 29.091 | 1.00 | 0.00 | 3A7 |
| ATOM | 1674 | O   | LYS | 251 | 42.946 | -24.559 | 29.945 | 1.00 | 0.00 | 3A7 |
| ATOM | 1675 | N   | SER | 252 | 40.996 | -24.057 | 28.942 | 1.00 | 0.00 | 3A7 |
| ATOM | 1676 | CA  | SER | 252 | 40.169 | -24.912 | 29.776 | 1.00 | 0.00 | 3A7 |
| ATOM | 1677 | CB  | SER | 252 | 38.679 | -24.780 | 29.422 | 1.00 | 0.00 | 3A7 |
| ATOM | 1678 | OG  | SER | 252 | 38.257 | -23.431 | 29.562 | 1.00 | 0.00 | 3A7 |
| ATOM | 1679 | C   | SER | 252 | 40.543 | -26.371 | 29.662 | 1.00 | 0.00 | 3A7 |
| ATOM | 1680 | O   | SER | 252 | 40.637 | -27.089 | 30.653 | 1.00 | 0.00 | 3A7 |
| ATOM | 1681 | N   | VAL | 253 | 40.836 | -26.832 | 28.425 | 1.00 | 0.00 | 3A7 |
| ATOM | 1682 | CA  | VAL | 253 | 41.211 | -28.203 | 28.125 | 1.00 | 0.00 | 3A7 |
| ATOM | 1683 | CB  | VAL | 253 | 41.292 | -28.416 | 26.609 | 1.00 | 0.00 | 3A7 |
| ATOM | 1684 | CG1 | VAL | 253 | 41.865 | -29.803 | 26.237 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1685 | CG2 | VAL | 253 | 39.886 | -28.264 | 25.997 | 1.00 | 0.00 | 3A7 |
| ATOM | 1686 | C   | VAL | 253 | 42.532 | -28.553 | 28.758 | 1.00 | 0.00 | 3A7 |
| ATOM | 1687 | O   | VAL | 253 | 42.684 | -29.586 | 29.404 | 1.00 | 0.00 | 3A7 |
| ATOM | 1688 | N   | LYS | 254 | 43.518 | -27.644 | 28.616 | 1.00 | 0.00 | 3A7 |
| ATOM | 1689 | CA  | LYS | 254 | 44.842 | -27.794 | 29.162 | 1.00 | 0.00 | 3A7 |
| ATOM | 1690 | CB  | LYS | 254 | 45.735 | -26.640 | 28.706 | 1.00 | 0.00 | 3A7 |
| ATOM | 1691 | CG  | LYS | 254 | 47.220 | -26.788 | 29.086 | 1.00 | 0.00 | 3A7 |
| ATOM | 1692 | CD  | LYS | 254 | 48.143 | -25.705 | 28.496 | 1.00 | 0.00 | 3A7 |
| ATOM | 1693 | CE  | LYS | 254 | 48.079 | -24.338 | 29.199 | 1.00 | 0.00 | 3A7 |
| ATOM | 1694 | NZ  | LYS | 254 | 46.811 | -23.622 | 28.925 | 1.00 | 0.00 | 3A7 |
| ATOM | 1695 | C   | LYS | 254 | 44.830 | -27.834 | 30.665 | 1.00 | 0.00 | 3A7 |
| ATOM | 1696 | O   | LYS | 254 | 45.412 | -28.728 | 31.270 | 1.00 | 0.00 | 3A7 |
| ATOM | 1697 | N   | GLN | 255 | 44.098 | -26.892 | 31.313 | 1.00 | 0.00 | 3A7 |
| ATOM | 1698 | CA  | GLN | 255 | 43.943 | -26.855 | 32.753 | 1.00 | 0.00 | 3A7 |
| ATOM | 1699 | CB  | GLN | 255 | 43.122 | -25.635 | 33.238 | 1.00 | 0.00 | 3A7 |
| ATOM | 1700 | CG  | GLN | 255 | 43.863 | -24.302 | 33.045 | 1.00 | 0.00 | 3A7 |
| ATOM | 1701 | CD  | GLN | 255 | 42.977 | -23.153 | 33.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 1702 | OE1 | GLN | 255 | 43.332 | -22.444 | 34.484 | 1.00 | 0.00 | 3A7 |
| ATOM | 1703 | NE2 | GLN | 255 | 41.801 | -22.974 | 32.860 | 1.00 | 0.00 | 3A7 |
| ATOM | 1704 | C   | GLN | 255 | 43.283 | -28.104 | 33.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 1705 | O   | GLN | 255 | 43.599 | -28.568 | 34.372 | 1.00 | 0.00 | 3A7 |
| ATOM | 1706 | N   | ILE | 256 | 42.375 | -28.710 | 32.490 | 1.00 | 0.00 | 3A7 |
| ATOM | 1707 | CA  | ILE | 256 | 41.679 | -29.907 | 32.888 | 1.00 | 0.00 | 3A7 |
| ATOM | 1708 | CB  | ILE | 256 | 40.404 | -30.098 | 32.072 | 1.00 | 0.00 | 3A7 |
| ATOM | 1709 | CG2 | ILE | 256 | 40.068 | -31.597 | 31.831 | 1.00 | 0.00 | 3A7 |
| ATOM | 1710 | CG1 | ILE | 256 | 39.198 | -29.508 | 32.862 | 1.00 | 0.00 | 3A7 |
| ATOM | 1711 | CD  | ILE | 256 | 39.270 | -28.036 | 33.277 | 1.00 | 0.00 | 3A7 |
| ATOM | 1712 | C   | ILE | 256 | 42.566 | -31.136 | 32.826 | 1.00 | 0.00 | 3A7 |
| ATOM | 1713 | O   | ILE | 256 | 42.411 | -32.060 | 33.627 | 1.00 | 0.00 | 3A7 |
| ATOM | 1714 | N   | LYS | 257 | 43.535 | -31.169 | 31.881 | 1.00 | 0.00 | 3A7 |
| ATOM | 1715 | CA  | LYS | 257 | 44.464 | -32.272 | 31.759 | 1.00 | 0.00 | 3A7 |
| ATOM | 1716 | CB  | LYS | 257 | 45.216 | -32.240 | 30.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 1717 | CG  | LYS | 257 | 44.304 | -32.548 | 29.218 | 1.00 | 0.00 | 3A7 |
| ATOM | 1718 | CD  | LYS | 257 | 45.027 | -32.676 | 27.864 | 1.00 | 0.00 | 3A7 |
| ATOM | 1719 | CE  | LYS | 257 | 45.583 | -31.365 | 27.283 | 1.00 | 0.00 | 3A7 |
| ATOM | 1720 | NZ  | LYS | 257 | 46.799 | -30.908 | 27.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 1721 | C   | LYS | 257 | 45.489 | -32.284 | 32.873 | 1.00 | 0.00 | 3A7 |
| ATOM | 1722 | O   | LYS | 257 | 45.944 | -33.343 | 33.303 | 1.00 | 0.00 | 3A7 |
| ATOM | 1723 | N   | GLU | 258 | 45.856 | -31.083 | 33.378 | 1.00 | 0.00 | 3A7 |
| ATOM | 1724 | CA  | GLU | 258 | 46.817 | -30.925 | 34.446 | 1.00 | 0.00 | 3A7 |
| ATOM | 1725 | CB  | GLU | 258 | 47.454 | -29.519 | 34.428 | 1.00 | 0.00 | 3A7 |
| ATOM | 1726 | CG  | GLU | 258 | 48.242 | -29.217 | 33.141 | 1.00 | 0.00 | 3A7 |
| ATOM | 1727 | CD  | GLU | 258 | 49.402 | -30.199 | 33.003 | 1.00 | 0.00 | 3A7 |
| ATOM | 1728 | OE1 | GLU | 258 | 50.286 | -30.202 | 33.900 | 1.00 | 0.00 | 3A7 |
| ATOM | 1729 | OE2 | GLU | 258 | 49.418 | -30.958 | 31.997 | 1.00 | 0.00 | 3A7 |
| ATOM | 1730 | C   | GLU | 258 | 46.174 | -31.151 | 35.797 | 1.00 | 0.00 | 3A7 |
| ATOM | 1731 | O   | GLU | 258 | 46.851 | -31.501 | 36.763 | 1.00 | 0.00 | 3A7 |
| ATOM | 1732 | N   | GLY | 259 | 44.829 | -30.971 | 35.870 | 1.00 | 0.00 | 3A7 |
| ATOM | 1733 | CA  | GLY | 259 | 44.026 | -31.194 | 37.052 | 1.00 | 0.00 | 3A7 |
| ATOM | 1734 | C   | GLY | 259 | 43.490 | -32.598 | 37.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 1735 | O   | GLY | 259 | 44.004 | -33.461 | 36.340 | 1.00 | 0.00 | 3A7 |
| ATOM | 1736 | N   | ARG | 260 | 42.444 | -32.842 | 37.887 | 1.00 | 0.00 | 3A7 |
| ATOM | 1737 | CA  | ARG | 260 | 41.787 | -34.118 | 38.133 | 1.00 | 0.00 | 3A7 |
| ATOM | 1738 | CB  | ARG | 260 | 41.489 | -34.954 | 36.853 | 1.00 | 0.00 | 3A7 |
| ATOM | 1739 | CG  | ARG | 260 | 40.639 | -36.233 | 37.027 | 1.00 | 0.00 | 3A7 |
| ATOM | 1740 | CD  | ARG | 260 | 39.172 | -36.004 | 37.425 | 1.00 | 0.00 | 3A7 |
| ATOM | 1741 | NE  | ARG | 260 | 39.105 | -35.667 | 38.882 | 1.00 | 0.00 | 3A7 |
| ATOM | 1742 | CZ  | ARG | 260 | 37.949 | -35.260 | 39.486 | 1.00 | 0.00 | 3A7 |
| ATOM | 1743 | NH1 | ARG | 260 | 37.967 | -34.927 | 40.809 | 1.00 | 0.00 | 3A7 |
| ATOM | 1744 | NH2 | ARG | 260 | 36.784 | -35.174 | 38.781 | 1.00 | 0.00 | 3A7 |
| ATOM | 1745 | C   | ARG | 260 | 42.631 | -34.898 | 39.116 | 1.00 | 0.00 | 3A7 |
| ATOM | 1746 | O   | ARG | 260 | 43.344 | -35.831 | 38.749 | 1.00 | 0.00 | 3A7 |
| ATOM | 1747 | N   | LEU | 261 | 42.581 | -34.475 | 40.403 | 1.00 | 0.00 | 3A7 |
| ATOM | 1748 | CA  | LEU | 261 | 43.473 | -34.943 | 41.438 | 1.00 | 0.00 | 3A7 |
| ATOM | 1749 | CB  | LEU | 261 | 44.463 | -33.853 | 41.945 | 1.00 | 0.00 | 3A7 |
| ATOM | 1750 | CG  | LEU | 261 | 43.883 | -32.584 | 42.630 | 1.00 | 0.00 | 3A7 |
| ATOM | 1751 | CD1 | LEU | 261 | 45.023 | -31.737 | 43.230 | 1.00 | 0.00 | 3A7 |
| ATOM | 1752 | CD2 | LEU | 261 | 43.009 | -31.708 | 41.709 | 1.00 | 0.00 | 3A7 |
| ATOM | 1753 | C   | LEU | 261 | 42.675 | -35.510 | 42.582 | 1.00 | 0.00 | 3A7 |
| ATOM | 1754 | O   | LEU | 261 | 43.042 | -36.544 | 43.138 | 1.00 | 0.00 | 3A7 |
| ATOM | 1755 | N   | LYS | 262 | 41.569 | -34.835 | 42.973 | 1.00 | 0.00 | 3A7 |
| ATOM | 1756 | CA  | LYS | 262 | 40.788 | -35.239 | 44.117 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1757 | CB  | LYS | 262 | 41.421 | -34.790 | 45.462 | 1.00 | 0.00 | 3A7 |
| ATOM | 1758 | CG  | LYS | 262 | 40.810 | -35.454 | 46.708 | 1.00 | 0.00 | 3A7 |
| ATOM | 1759 | CD  | LYS | 262 | 41.515 | -35.043 | 48.009 | 1.00 | 0.00 | 3A7 |
| ATOM | 1760 | CE  | LYS | 262 | 41.066 | -35.853 | 49.233 | 1.00 | 0.00 | 3A7 |
| ATOM | 1761 | NZ  | LYS | 262 | 39.611 | -35.711 | 49.468 | 1.00 | 0.00 | 3A7 |
| ATOM | 1762 | C   | LYS | 262 | 39.442 | -34.600 | 43.941 | 1.00 | 0.00 | 3A7 |
| ATOM | 1763 | O   | LYS | 262 | 39.325 | -33.548 | 43.313 | 1.00 | 0.00 | 3A7 |
| ATOM | 1764 | N   | GLU | 263 | 38.381 | -35.233 | 44.510 | 1.00 | 0.00 | 3A7 |
| ATOM | 1765 | CA  | GLU | 263 | 37.009 | -34.774 | 44.438 | 1.00 | 0.00 | 3A7 |
| ATOM | 1766 | CB  | GLU | 263 | 36.001 | -35.949 | 44.396 | 1.00 | 0.00 | 3A7 |
| ATOM | 1767 | CG  | GLU | 263 | 36.178 | -36.837 | 43.152 | 1.00 | 0.00 | 3A7 |
| ATOM | 1768 | CD  | GLU | 263 | 35.147 | -37.964 | 43.149 | 1.00 | 0.00 | 3A7 |
| ATOM | 1769 | OE1 | GLU | 263 | 34.322 | -38.035 | 44.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 1770 | OE2 | GLU | 263 | 35.174 | -38.773 | 42.183 | 1.00 | 0.00 | 3A7 |
| ATOM | 1771 | C   | GLU | 263 | 36.698 | -33.900 | 45.630 | 1.00 | 0.00 | 3A7 |
| ATOM | 1772 | O   | GLU | 263 | 35.910 | -34.265 | 46.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 1773 | N   | THR | 264 | 37.333 | -32.704 | 45.670 | 1.00 | 0.00 | 3A7 |
| ATOM | 1774 | CA  | THR | 264 | 37.170 | -31.721 | 46.715 | 1.00 | 0.00 | 3A7 |
| ATOM | 1775 | CB  | THR | 264 | 38.280 | -31.765 | 47.757 | 1.00 | 0.00 | 3A7 |
| ATOM | 1776 | OG1 | THR | 264 | 38.329 | -33.054 | 48.352 | 1.00 | 0.00 | 3A7 |
| ATOM | 1777 | CG2 | THR | 264 | 38.047 | -30.721 | 48.870 | 1.00 | 0.00 | 3A7 |
| ATOM | 1778 | C   | THR | 264 | 37.164 | -30.395 | 46.003 | 1.00 | 0.00 | 3A7 |
| ATOM | 1779 | O   | THR | 264 | 36.480 | -29.458 | 46.415 | 1.00 | 0.00 | 3A7 |
| ATOM | 1780 | N   | GLN | 265 | 37.940 | -30.300 | 44.890 | 1.00 | 0.00 | 3A7 |
| ATOM | 1781 | CA  | GLN | 265 | 38.063 | -29.123 | 44.052 | 1.00 | 0.00 | 3A7 |
| ATOM | 1782 | CB  | GLN | 265 | 39.417 | -29.038 | 43.298 | 1.00 | 0.00 | 3A7 |
| ATOM | 1783 | CG  | GLN | 265 | 40.645 | -28.808 | 44.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 1784 | CD  | GLN | 265 | 40.965 | -30.055 | 45.032 | 1.00 | 0.00 | 3A7 |
| ATOM | 1785 | OE1 | GLN | 265 | 41.070 | -31.165 | 44.497 | 1.00 | 0.00 | 3A7 |
| ATOM | 1786 | NE2 | GLN | 265 | 41.132 | -29.849 | 46.374 | 1.00 | 0.00 | 3A7 |
| ATOM | 1787 | C   | GLN | 265 | 36.953 | -29.140 | 43.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 1788 | O   | GLN | 265 | 36.287 | -28.132 | 42.802 | 1.00 | 0.00 | 3A7 |
| ATOM | 1789 | N   | LYS | 266 | 36.738 | -30.320 | 42.404 | 1.00 | 0.00 | 3A7 |
| ATOM | 1790 | CA  | LYS | 266 | 35.642 | -30.556 | 41.500 | 1.00 | 0.00 | 3A7 |
| ATOM | 1791 | CB  | LYS | 266 | 36.035 | -30.452 | 40.002 | 1.00 | 0.00 | 3A7 |
| ATOM | 1792 | CG  | LYS | 266 | 37.305 | -31.216 | 39.591 | 1.00 | 0.00 | 3A7 |
| ATOM | 1793 | CD  | LYS | 266 | 37.703 | -30.959 | 38.129 | 1.00 | 0.00 | 3A7 |
| ATOM | 1794 | CE  | LYS | 266 | 38.982 | -31.700 | 37.724 | 1.00 | 0.00 | 3A7 |
| ATOM | 1795 | NZ  | LYS | 266 | 39.346 | -31.401 | 36.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 1796 | C   | LYS | 266 | 35.129 | -31.922 | 41.858 | 1.00 | 0.00 | 3A7 |
| ATOM | 1797 | O   | LYS | 266 | 35.796 | -32.934 | 41.655 | 1.00 | 0.00 | 3A7 |
| ATOM | 1798 | N   | HIS | 267 | 33.902 | -31.966 | 42.437 | 1.00 | 0.00 | 3A7 |
| ATOM | 1799 | CA  | HIS | 267 | 33.272 | -33.168 | 42.940 | 1.00 | 0.00 | 3A7 |
| ATOM | 1800 | ND1 | HIS | 267 | 32.504 | -35.052 | 45.499 | 1.00 | 0.00 | 3A7 |
| ATOM | 1801 | CG  | HIS | 267 | 31.780 | -34.098 | 44.815 | 1.00 | 0.00 | 3A7 |
| ATOM | 1802 | CB  | HIS | 267 | 32.380 | -32.874 | 44.174 | 1.00 | 0.00 | 3A7 |
| ATOM | 1803 | NE2 | HIS | 267 | 30.385 | -35.724 | 45.524 | 1.00 | 0.00 | 3A7 |
| ATOM | 1804 | CD2 | HIS | 267 | 30.489 | -34.526 | 44.840 | 1.00 | 0.00 | 3A7 |
| ATOM | 1805 | CE1 | HIS | 267 | 31.620 | -35.999 | 45.901 | 1.00 | 0.00 | 3A7 |
| ATOM | 1806 | C   | HIS | 267 | 32.435 | -33.802 | 41.858 | 1.00 | 0.00 | 3A7 |
| ATOM | 1807 | O   | HIS | 267 | 32.255 | -35.018 | 41.834 | 1.00 | 0.00 | 3A7 |
| ATOM | 1808 | N   | ARG | 268 | 31.909 | -32.963 | 40.929 | 1.00 | 0.00 | 3A7 |
| ATOM | 1809 | CA  | ARG | 268 | 31.110 | -33.390 | 39.804 | 1.00 | 0.00 | 3A7 |
| ATOM | 1810 | CB  | ARG | 268 | 29.939 | -32.419 | 39.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 1811 | CG  | ARG | 268 | 30.357 | -30.974 | 39.172 | 1.00 | 0.00 | 3A7 |
| ATOM | 1812 | CD  | ARG | 268 | 29.154 | -30.049 | 38.948 | 1.00 | 0.00 | 3A7 |
| ATOM | 1813 | NE  | ARG | 268 | 29.664 | -28.690 | 38.573 | 1.00 | 0.00 | 3A7 |
| ATOM | 1814 | CZ  | ARG | 268 | 28.818 | -27.637 | 38.353 | 1.00 | 0.00 | 3A7 |
| ATOM | 1815 | NH1 | ARG | 268 | 29.328 | -26.423 | 37.993 | 1.00 | 0.00 | 3A7 |
| ATOM | 1816 | NH2 | ARG | 268 | 27.470 | -27.791 | 38.491 | 1.00 | 0.00 | 3A7 |
| ATOM | 1817 | C   | ARG | 268 | 31.997 | -33.501 | 38.593 | 1.00 | 0.00 | 3A7 |
| ATOM | 1818 | O   | ARG | 268 | 33.012 | -32.813 | 38.485 | 1.00 | 0.00 | 3A7 |
| ATOM | 1819 | N   | VAL | 269 | 31.604 | -34.383 | 37.643 | 1.00 | 0.00 | 3A7 |
| ATOM | 1820 | CA  | VAL | 269 | 32.279 | -34.566 | 36.378 | 1.00 | 0.00 | 3A7 |
| ATOM | 1821 | CB  | VAL | 269 | 32.595 | -36.021 | 36.063 | 1.00 | 0.00 | 3A7 |
| ATOM | 1822 | CG1 | VAL | 269 | 33.733 | -36.473 | 37.001 | 1.00 | 0.00 | 3A7 |
| ATOM | 1823 | CG2 | VAL | 269 | 31.340 | -36.903 | 36.220 | 1.00 | 0.00 | 3A7 |
| ATOM | 1824 | C   | VAL | 269 | 31.408 | -33.947 | 35.315 | 1.00 | 0.00 | 3A7 |
| ATOM | 1825 | O   | VAL | 269 | 30.217 | -33.712 | 35.519 | 1.00 | 0.00 | 3A7 |
| ATOM | 1826 | N   | ASP | 270 | 32.030 | -33.642 | 34.156 | 1.00 | 0.00 | 3A7 |
| ATOM | 1827 | CA  | ASP | 270 | 31.450 | -32.836 | 33.096 | 1.00 | 0.00 | 3A7 |
| ATOM | 1828 | CB  | ASP | 270 | 31.980 | -31.399 | 33.132 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1829 | CG  | ASP | 270 | 33.510 | -31.368 | 33.034 | 1.00 | 0.00 | 3A7 |
| ATOM | 1830 | OD1 | ASP | 270 | 34.013 | -30.868 | 31.995 | 1.00 | 0.00 | 3A7 |
| ATOM | 1831 | OD2 | ASP | 270 | 34.191 | -31.809 | 33.998 | 1.00 | 0.00 | 3A7 |
| ATOM | 1832 | C   | ASP | 270 | 31.710 | -33.510 | 31.781 | 1.00 | 0.00 | 3A7 |
| ATOM | 1833 | O   | ASP | 270 | 32.369 | -34.547 | 31.709 | 1.00 | 0.00 | 3A7 |
| ATOM | 1834 | N   | PHE | 271 | 31.187 | -32.915 | 30.684 | 1.00 | 0.00 | 3A7 |
| ATOM | 1835 | CA  | PHE | 271 | 31.302 | -33.474 | 29.357 | 1.00 | 0.00 | 3A7 |
| ATOM | 1836 | CB  | PHE | 271 | 30.407 | -32.722 | 28.356 | 1.00 | 0.00 | 3A7 |
| ATOM | 1837 | CG  | PHE | 271 | 30.344 | -33.517 | 27.080 | 1.00 | 0.00 | 3A7 |
| ATOM | 1838 | CD1 | PHE | 271 | 30.012 | -34.875 | 27.101 | 1.00 | 0.00 | 3A7 |
| ATOM | 1839 | CD2 | PHE | 271 | 30.758 | -32.938 | 25.887 | 1.00 | 0.00 | 3A7 |
| ATOM | 1840 | CE1 | PHE | 271 | 30.211 | -35.660 | 25.972 | 1.00 | 0.00 | 3A7 |
| ATOM | 1841 | CE2 | PHE | 271 | 30.870 | -33.707 | 24.737 | 1.00 | 0.00 | 3A7 |
| ATOM | 1842 | CZ  | PHE | 271 | 30.646 | -35.078 | 24.793 | 1.00 | 0.00 | 3A7 |
| ATOM | 1843 | C   | PHE | 271 | 32.719 | -33.478 | 28.848 | 1.00 | 0.00 | 3A7 |
| ATOM | 1844 | O   | PHE | 271 | 33.150 | -34.431 | 28.204 | 1.00 | 0.00 | 3A7 |
| ATOM | 1845 | N   | LEU | 272 | 33.494 | -32.417 | 29.146 | 1.00 | 0.00 | 3A7 |
| ATOM | 1846 | CA  | LEU | 272 | 34.866 | -32.326 | 28.716 | 1.00 | 0.00 | 3A7 |
| ATOM | 1847 | CB  | LEU | 272 | 35.455 | -30.979 | 29.100 | 1.00 | 0.00 | 3A7 |
| ATOM | 1848 | CG  | LEU | 272 | 36.816 | -30.698 | 28.482 | 1.00 | 0.00 | 3A7 |
| ATOM | 1849 | CD1 | LEU | 272 | 36.864 | -29.210 | 28.078 | 1.00 | 0.00 | 3A7 |
| ATOM | 1850 | CD2 | LEU | 272 | 38.027 | -31.011 | 29.363 | 1.00 | 0.00 | 3A7 |
| ATOM | 1851 | C   | LEU | 272 | 35.735 | -33.394 | 29.311 | 1.00 | 0.00 | 3A7 |
| ATOM | 1852 | O   | LEU | 272 | 36.573 | -33.979 | 28.634 | 1.00 | 0.00 | 3A7 |
| ATOM | 1853 | N   | GLN | 273 | 35.522 | -33.712 | 30.606 | 1.00 | 0.00 | 3A7 |
| ATOM | 1854 | CA  | GLN | 273 | 36.255 | -34.750 | 31.288 | 1.00 | 0.00 | 3A7 |
| ATOM | 1855 | CB  | GLN | 273 | 35.890 | -34.805 | 32.788 | 1.00 | 0.00 | 3A7 |
| ATOM | 1856 | CG  | GLN | 273 | 36.853 | -35.634 | 33.658 | 1.00 | 0.00 | 3A7 |
| ATOM | 1857 | CD  | GLN | 273 | 38.222 | -34.946 | 33.686 | 1.00 | 0.00 | 3A7 |
| ATOM | 1858 | OE1 | GLN | 273 | 38.361 | -33.845 | 34.234 | 1.00 | 0.00 | 3A7 |
| ATOM | 1859 | NE2 | GLN | 273 | 39.247 | -35.617 | 33.079 | 1.00 | 0.00 | 3A7 |
| ATOM | 1860 | C   | GLN | 273 | 35.971 | -36.088 | 30.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 1861 | O   | GLN | 273 | 36.882 | -36.879 | 30.456 | 1.00 | 0.00 | 3A7 |
| ATOM | 1862 | N   | LEU | 274 | 34.685 | -36.340 | 30.310 | 1.00 | 0.00 | 3A7 |
| ATOM | 1863 | CA  | LEU | 274 | 34.245 | -37.560 | 29.669 | 1.00 | 0.00 | 3A7 |
| ATOM | 1864 | CB  | LEU | 274 | 32.718 | -37.631 | 29.471 | 1.00 | 0.00 | 3A7 |
| ATOM | 1865 | CG  | LEU | 274 | 31.891 | -37.798 | 30.761 | 1.00 | 0.00 | 3A7 |
| ATOM | 1866 | CD1 | LEU | 274 | 30.398 | -37.811 | 30.394 | 1.00 | 0.00 | 3A7 |
| ATOM | 1867 | CD2 | LEU | 274 | 32.273 | -39.060 | 31.558 | 1.00 | 0.00 | 3A7 |
| ATOM | 1868 | C   | LEU | 274 | 34.854 | -37.729 | 28.302 | 1.00 | 0.00 | 3A7 |
| ATOM | 1869 | O   | LEU | 274 | 35.232 | -38.832 | 27.930 | 1.00 | 0.00 | 3A7 |
| ATOM | 1870 | N   | MET | 275 | 35.003 | -36.636 | 27.521 | 1.00 | 0.00 | 3A7 |
| ATOM | 1871 | CA  | MET | 275 | 35.607 | -36.702 | 26.211 | 1.00 | 0.00 | 3A7 |
| ATOM | 1872 | CB  | MET | 275 | 35.400 | -35.428 | 25.399 | 1.00 | 0.00 | 3A7 |
| ATOM | 1873 | CG  | MET | 275 | 33.958 | -35.154 | 24.962 | 1.00 | 0.00 | 3A7 |
| ATOM | 1874 | SD  | MET | 275 | 33.857 | -33.829 | 23.713 | 1.00 | 0.00 | 3A7 |
| ATOM | 1875 | CE  | MET | 275 | 34.315 | -32.435 | 24.786 | 1.00 | 0.00 | 3A7 |
| ATOM | 1876 | C   | MET | 275 | 37.090 | -36.951 | 26.286 | 1.00 | 0.00 | 3A7 |
| ATOM | 1877 | Q   | MET | 275 | 37.642 | -37.666 | 25.458 | 1.00 | 0.00 | 3A7 |
| ATOM | 1878 | N   | ILE | 276 | 37.778 | -36.381 | 27.305 | 1.00 | 0.00 | 3A7 |
| ATOM | 1879 | CA  | ILE | 276 | 39.215 | -36.516 | 27.488 | 1.00 | 0.00 | 3A7 |
| ATOM | 1880 | CB  | ILE | 276 | 39.723 | -35.567 | 28.575 | 1.00 | 0.00 | 3A7 |
| ATOM | 1881 | CG2 | ILE | 276 | 41.140 | -35.906 | 29.105 | 1.00 | 0.00 | 3A7 |
| ATOM | 1882 | CG1 | ILE | 276 | 39.717 | -34.100 | 28.081 | 1.00 | 0.00 | 3A7 |
| ATOM | 1883 | CD  | ILE | 276 | 40.767 | -33.779 | 27.011 | 1.00 | 0.00 | 3A7 |
| ATOM | 1884 | C   | ILE | 276 | 39.615 | -37.926 | 27.833 | 1.00 | 0.00 | 3A7 |
| ATOM | 1885 | O   | ILE | 276 | 40.701 | -38.375 | 27.476 | 1.00 | 0.00 | 3A7 |
| ATOM | 1886 | N   | ASP | 277 | 38.749 | -38.659 | 28.548 | 1.00 | 0.00 | 3A7 |
| ATOM | 1887 | CA  | ASP | 277 | 39.133 | -39.958 | 29.016 | 1.00 | 0.00 | 3A7 |
| ATOM | 1888 | CB  | ASP | 277 | 38.914 | -40.156 | 30.516 | 1.00 | 0.00 | 3A7 |
| ATOM | 1889 | CG  | ASP | 277 | 39.827 | -39.210 | 31.302 | 1.00 | 0.00 | 3A7 |
| ATOM | 1890 | OD1 | ASP | 277 | 40.999 | -39.021 | 30.882 | 1.00 | 0.00 | 3A7 |
| ATOM | 1891 | OD2 | ASP | 277 | 39.351 | -38.657 | 32.329 | 1.00 | 0.00 | 3A7 |
| ATOM | 1892 | C   | ASP | 277 | 38.346 | -41.070 | 28.476 | 1.00 | 0.00 | 3A7 |
| ATOM | 1893 | O   | ASP | 277 | 38.933 | -42.095 | 28.164 | 1.00 | 0.00 | 3A7 |
| ATOM | 1894 | N   | SER | 278 | 36.987 | -41.031 | 28.602 | 1.00 | 0.00 | 3A7 |
| ATOM | 1895 | CA  | SER | 278 | 36.186 | -42.176 | 29.071 | 1.00 | 0.00 | 3A7 |
| ATOM | 1896 | CB  | SER | 278 | 34.677 | -41.818 | 29.196 | 1.00 | 0.00 | 3A7 |
| ATOM | 1897 | OG  | SER | 278 | 34.091 | -41.424 | 27.961 | 1.00 | 0.00 | 3A7 |
| ATOM | 1898 | C   | SER | 278 | 36.329 | -43.499 | 28.318 | 1.00 | 0.00 | 3A7 |
| ATOM | 1899 | O   | SER | 278 | 35.567 | -43.792 | 27.399 | 1.00 | 0.00 | 3A7 |
| ATOM | 1900 | N   | GLN | 279 | 37.341 | -44.307 | 28.750 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1901 | CA  | GLN | 279 | 37.851 | -45.539 | 28.167 | 1.00 | 0.00 | 3A7 |
| ATOM | 1902 | CB  | GLN | 279 | 36.793 | -46.503 | 27.561 | 1.00 | 0.00 | 3A7 |
| ATOM | 1903 | CG  | GLN | 279 | 35.768 | -47.000 | 28.593 | 1.00 | 0.00 | 3A7 |
| ATOM | 1904 | CD  | GLN | 279 | 34.775 | -47.928 | 27.887 | 1.00 | 0.00 | 3A7 |
| ATOM | 1905 | OE1 | GLN | 279 | 35.143 | -49.016 | 27.428 | 1.00 | 0.00 | 3A7 |
| ATOM | 1906 | NE2 | GLN | 279 | 33.487 | -47.472 | 27.805 | 1.00 | 0.00 | 3A7 |
| ATOM | 1907 | C   | GLN | 279 | 38.889 | -45.204 | 27.116 | 1.00 | 0.00 | 3A7 |
| ATOM | 1908 | O   | GLN | 279 | 38.687 | -45.481 | 25.937 | 1.00 | 0.00 | 3A7 |
| ATOM | 1909 | N   | ASN | 280 | 40.027 | -44.587 | 27.552 | 1.00 | 0.00 | 3A7 |
| ATOM | 1910 | CA  | ASN | 280 | 41.202 | -44.166 | 26.787 | 1.00 | 0.00 | 3A7 |
| ATOM | 1911 | CB  | ASN | 280 | 42.008 | -45.358 | 26.209 | 1.00 | 0.00 | 3A7 |
| ATOM | 1912 | CG  | ASN | 280 | 42.430 | -46.296 | 27.347 | 1.00 | 0.00 | 3A7 |
| ATOM | 1913 | OD1 | ASN | 280 | 41.937 | -47.427 | 27.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 1914 | ND2 | ASN | 280 | 43.366 | -45.803 | 28.213 | 1.00 | 0.00 | 3A7 |
| ATOM | 1915 | C   | ASN | 280 | 40.890 | -43.183 | 25.664 | 1.00 | 0.00 | 3A7 |
| ATOM | 1916 | O   | ASN | 280 | 40.934 | -43.532 | 24.487 | 1.00 | 0.00 | 3A7 |
| ATOM | 1917 | N   | SER | 281 | 40.551 | -41.923 | 26.053 | 1.00 | 0.00 | 3A7 |
| ATOM | 1918 | CA  | SER | 281 | 40.076 | -40.803 | 25.252 | 1.00 | 0.00 | 3A7 |
| ATOM | 1919 | CB  | SER | 281 | 40.924 | -40.513 | 23.986 | 1.00 | 0.00 | 3A7 |
| ATOM | 1920 | OG  | SER | 281 | 42.283 | -40.298 | 24.340 | 1.00 | 0.00 | 3A7 |
| ATOM | 1921 | C   | SER | 281 | 38.621 | -40.951 | 24.837 | 1.00 | 0.00 | 3A7 |
| ATOM | 1922 | O   | SER | 281 | 38.131 | -40.172 | 24.021 | 1.00 | 0.00 | 3A7 |
| ATOM | 1923 | N   | LYS | 282 | 37.924 | -42.020 | 25.342 | 1.00 | 0.00 | 3A7 |
| ATOM | 1924 | CA  | LYS | 282 | 36.818 | -42.723 | 24.707 | 1.00 | 0.00 | 3A7 |
| ATOM | 1925 | CB  | LYS | 282 | 35.459 | -42.013 | 24.620 | 1.00 | 0.00 | 3A7 |
| ATOM | 1926 | CG  | LYS | 282 | 34.288 | -42.957 | 24.294 | 1.00 | 0.00 | 3A7 |
| ATOM | 1927 | CD  | LYS | 282 | 32.914 | -42.336 | 24.590 | 1.00 | 0.00 | 3A7 |
| ATOM | 1928 | CE  | LYS | 282 | 31.744 | -43.301 | 24.357 | 1.00 | 0.00 | 3A7 |
| ATOM | 1929 | NZ  | LYS | 282 | 31.691 | -43.746 | 22.946 | 1.00 | 0.00 | 3A7 |
| ATOM | 1930 | C   | LYS | 282 | 37.194 | -43.157 | 23.334 | 1.00 | 0.00 | 3A7 |
| ATOM | 1931 | O   | LYS | 282 | 37.082 | -42.407 | 22.364 | 1.00 | 0.00 | 3A7 |
| ATOM | 1932 | N   | ASP | 283 | 37.706 | -44.392 | 23.270 | 1.00 | 0.00 | 3A7 |
| ATOM | 1933 | CA  | ASP | 283 | 38.125 | -44.964 | 22.041 | 1.00 | 0.00 | 3A7 |
| ATOM | 1934 | CB  | ASP | 283 | 39.663 | -45.088 | 21.918 | 1.00 | 0.00 | 3A7 |
| ATOM | 1935 | CG  | ASP | 283 | 40.442 | -46.002 | 22.880 | 1.00 | 0.00 | 3A7 |
| ATOM | 1936 | OD1 | ASP | 283 | 41.683 | -46.097 | 22.672 | 1.00 | 0.00 | 3A7 |
| ATOM | 1937 | OD2 | ASP | 283 | 39.853 | -46.604 | 23.810 | 1.00 | 0.00 | 3A7 |
| ATOM | 1938 | C   | ASP | 283 | 37.352 | -46.233 | 21.948 | 1.00 | 0.00 | 3A7 |
| ATOM | 1939 | O   | ASP | 283 | 37.675 | -47.232 | 22.581 | 1.00 | 0.00 | 3A7 |
| ATOM | 1940 | N   | SER | 284 | 36.258 | -46.198 | 21.157 | 1.00 | 0.00 | 3A7 |
| ATOM | 1941 | CA  | SER | 284 | 35.513 | -47.378 | 20.782 | 1.00 | 0.00 | 3A7 |
| ATOM | 1942 | CB  | SER | 284 | 34.115 | -47.009 | 20.210 | 1.00 | 0.00 | 3A7 |
| ATOM | 1943 | OG  | SER | 284 | 34.183 | -45.995 | 19.212 | 1.00 | 0.00 | 3A7 |
| ATOM | 1944 | C   | SER | 284 | 36.266 | -48.277 | 19.834 | 1.00 | 0.00 | 3A7 |
| ATOM | 1945 | O   | SER | 284 | 36.990 | -49.180 | 20.242 | 1.00 | 0.00 | 3A7 |
| ATOM | 1946 | N   | GLU | 285 | 36.113 | -48.092 | 18.521 | 1.00 | 0.00 | 3A7 |
| ATOM | 1947 | CA  | GLU | 285 | 36.639 | -49.081 | 17.634 | 1.00 | 0.00 | 3A7 |
| ATOM | 1948 | CB  | GLU | 285 | 35.795 | -49.213 | 16.369 | 1.00 | 0.00 | 3A7 |
| ATOM | 1949 | CG  | GLU | 285 | 35.628 | -47.895 | 15.591 | 1.00 | 0.00 | 3A7 |
| ATOM | 1950 | CD  | GLU | 285 | 34.752 | -48.143 | 14.367 | 1.00 | 0.00 | 3A7 |
| ATOM | 1951 | OE1 | GLU | 285 | 33.566 | -48.527 | 14.555 | 1.00 | 0.00 | 3A7 |
| ATOM | 1952 | OE2 | GLU | 285 | 35.255 | -47.948 | 13.228 | 1.00 | 0.00 | 3A7 |
| ATOM | 1953 | C   | GLU | 285 | 38.083 | -48.834 | 17.309 | 1.00 | 0.00 | 3A7 |
| ATOM | 1954 | O   | GLU | 285 | 38.621 | -49.477 | 16.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 1955 | N   | THR | 286 | 38.744 | -47.901 | 18.009 | 1.00 | 0.00 | 3A7 |
| ATOM | 1956 | CA  | THR | 286 | 40.099 | -47.398 | 17.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 1957 | CB  | THR | 286 | 41.251 | -48.366 | 17.728 | 1.00 | 0.00 | 3A7 |
| ATOM | 1958 | OG1 | THR | 286 | 41.071 | -49.460 | 18.620 | 1.00 | 0.00 | 3A7 |
| ATOM | 1959 | CG2 | THR | 286 | 42.623 | -47.726 | 18.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 1960 | C   | THR | 286 | 40.161 | -46.319 | 16.868 | 1.00 | 0.00 | 3A7 |
| ATOM | 1961 | O   | THR | 286 | 41.095 | -45.529 | 16.847 | 1.00 | 0.00 | 3A7 |
| ATOM | 1962 | N   | HIS | 287 | 39.201 | -46.294 | 15.904 | 1.00 | 0.00 | 3A7 |
| ATOM | 1963 | CA  | HIS | 287 | 39.294 | -45.529 | 14.676 | 1.00 | 0.00 | 3A7 |
| ATOM | 1964 | ND1 | HIS | 287 | 37.806 | -44.452 | 11.739 | 1.00 | 0.00 | 3A7 |
| ATOM | 1965 | CG  | HIS | 287 | 38.588 | -45.495 | 12.192 | 1.00 | 0.00 | 3A7 |
| ATOM | 1966 | CB  | HIS | 287 | 38.440 | -46.152 | 13.541 | 1.00 | 0.00 | 3A7 |
| ATOM | 1967 | NE2 | HIS | 287 | 39.260 | -44.903 | 10.120 | 1.00 | 0.00 | 3A7 |
| ATOM | 1968 | CD2 | HIS | 287 | 39.470 | -45.756 | 11.189 | 1.00 | 0.00 | 3A7 |
| ATOM | 1969 | CE1 | HIS | 287 | 38.251 | -44.140 | 10.497 | 1.00 | 0.00 | 3A7 |
| ATOM | 1970 | C   | HIS | 287 | 38.868 | -44.107 | 14.911 | 1.00 | 0.00 | 3A7 |
| ATOM | 1971 | O   | HIS | 287 | 37.679 | -43.797 | 14.904 | 1.00 | 0.00 | 3A7 |
| ATOM | 1972 | N   | LYS | 288 | 39.880 | -43.225 | 15.122 | 1.00 | 0.00 | 3A7 |



|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 1973 | CA  | LYS | 288 | 39.776 | -41.800 | 15.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 1974 | CB  | LYS | 288 | 38.889 | -41.036 | 14.340 | 1.00 | 0.00 | 3A7 |
| ATOM | 1975 | CG  | LYS | 288 | 39.415 | -41.157 | 12.901 | 1.00 | 0.00 | 3A7 |
| ATOM | 1976 | CD  | LYS | 288 | 38.528 | -40.437 | 11.877 | 1.00 | 0.00 | 3A7 |
| ATOM | 1977 | CE  | LYS | 288 | 39.036 | -40.557 | 10.434 | 1.00 | 0.00 | 3A7 |
| ATOM | 1978 | NZ  | LYS | 288 | 40.358 | -39.909 | 10.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 1979 | C   | LYS | 288 | 39.309 | -41.522 | 16.767 | 1.00 | 0.00 | 3A7 |
| ATOM | 1980 | O   | LYS | 288 | 38.116 | -41.380 | 17.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 1981 | N   | ALA | 289 | 40.290 | -41.406 | 17.701 | 1.00 | 0.00 | 3A7 |
| ATOM | 1982 | CA  | ALA | 289 | 40.092 | -40.977 | 19.070 | 1.00 | 0.00 | 3A7 |
| ATOM | 1983 | CB  | ALA | 289 | 41.158 | -41.545 | 20.027 | 1.00 | 0.00 | 3A7 |
| ATOM | 1984 | C   | ALA | 289 | 40.164 | -39.473 | 19.078 | 1.00 | 0.00 | 3A7 |
| ATOM | 1985 | O   | ALA | 289 | 40.670 | -38.875 | 18.128 | 1.00 | 0.00 | 3A7 |
| ATOM | 1986 | N   | LEU | 290 | 39.624 | -38.812 | 20.137 | 1.00 | 0.00 | 3A7 |
| ATOM | 1987 | CA  | LEU | 290 | 39.349 | -37.401 | 20.081 | 1.00 | 0.00 | 3A7 |
| ATOM | 1988 | CB  | LEU | 290 | 38.229 | -37.004 | 21.014 | 1.00 | 0.00 | 3A7 |
| ATOM | 1989 | CG  | LEU | 290 | 36.888 | -37.703 | 20.701 | 1.00 | 0.00 | 3A7 |
| ATOM | 1990 | CD1 | LEU | 290 | 35.892 | -37.512 | 21.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 1991 | CD2 | LEU | 290 | 36.312 | -37.221 | 19.355 | 1.00 | 0.00 | 3A7 |
| ATOM | 1992 | C   | LEU | 290 | 40.550 | -36.573 | 20.350 | 1.00 | 0.00 | 3A7 |
| ATOM | 1993 | O   | LEU | 290 | 41.191 | -36.642 | 21.390 | 1.00 | 0.00 | 3A7 |
| ATOM | 1994 | N   | SER | 291 | 40.854 | -35.731 | 19.352 | 1.00 | 0.00 | 3A7 |
| ATOM | 1995 | CA  | SER | 291 | 41.954 | -34.822 | 19.363 | 1.00 | 0.00 | 3A7 |
| ATOM | 1996 | CB  | SER | 291 | 42.455 | -34.592 | 17.928 | 1.00 | 0.00 | 3A7 |
| ATOM | 1997 | OG  | SER | 291 | 41.422 | -34.204 | 17.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 1998 | C   | SER | 291 | 41.471 | -33.540 | 19.957 | 1.00 | 0.00 | 3A7 |
| ATOM | 1999 | O   | SER | 291 | 40.275 | -33.273 | 19.991 | 1.00 | 0.00 | 3A7 |
| ATOM | 2000 | N   | ASP | 292 | 42.400 | -32.681 | 20.410 | 1.00 | 0.00 | 3A7 |
| ATOM | 2001 | CA  | ASP | 292 | 42.071 | -31.438 | 21.064 | 1.00 | 0.00 | 3A7 |
| ATOM | 2002 | CB  | ASP | 292 | 43.338 | -30.745 | 21.556 | 1.00 | 0.00 | 3A7 |
| ATOM | 2003 | CG  | ASP | 292 | 44.042 | -31.647 | 22.570 | 1.00 | 0.00 | 3A7 |
| ATOM | 2004 | OD1 | ASP | 292 | 43.426 | -31.941 | 23.629 | 1.00 | 0.00 | 3A7 |
| ATOM | 2005 | OD2 | ASP | 292 | 45.204 | -32.050 | 22.298 | 1.00 | 0.00 | 3A7 |
| ATOM | 2006 | C   | ASP | 292 | 41.334 | -30.471 | 20.170 | 1.00 | 0.00 | 3A7 |
| ATOM | 2007 | O   | ASP | 292 | 40.568 | -29.641 | 20.643 | 1.00 | 0.00 | 3A7 |
| ATOM | 2008 | N   | LEU | 293 | 41.506 | -30.616 | 18.834 | 1.00 | 0.00 | 3A7 |
| ATOM | 2009 | CA  | LEU | 293 | 40.836 | -29.795 | 17.858 | 1.00 | 0.00 | 3A7 |
| ATOM | 2010 | CB  | LEU | 293 | 41.527 | -29.876 | 16.490 | 1.00 | 0.00 | 3A7 |
| ATOM | 2011 | CG  | LEU | 293 | 43.011 | -29.436 | 16.506 | 1.00 | 0.00 | 3A7 |
| ATOM | 2012 | CD1 | LEU | 293 | 43.663 | -29.663 | 15.129 | 1.00 | 0.00 | 3A7 |
| ATOM | 2013 | CD2 | LEU | 293 | 43.189 | -27.976 | 16.965 | 1.00 | 0.00 | 3A7 |
| ATOM | 2014 | C   | LEU | 293 | 39.382 | -30.187 | 17.711 | 1.00 | 0.00 | 3A7 |
| ATOM | 2015 | O   | LEU | 293 | 38.493 | -29.340 | 17.738 | 1.00 | 0.00 | 3A7 |
| ATOM | 2016 | N   | GLU | 294 | 39.081 | -31.502 | 17.619 | 1.00 | 0.00 | 3A7 |
| ATOM | 2017 | CA  | GLU | 294 | 37.722 | -31.998 | 17.504 | 1.00 | 0.00 | 3A7 |
| ATOM | 2018 | CB  | GLU | 294 | 37.697 | -33.523 | 17.310 | 1.00 | 0.00 | 3A7 |
| ATOM | 2019 | CG  | GLU | 294 | 38.247 | -33.957 | 15.942 | 1.00 | 0.00 | 3A7 |
| ATOM | 2020 | CD  | GLU | 294 | 38.198 | -35.480 | 15.850 | 1.00 | 0.00 | 3A7 |
| ATOM | 2021 | OE1 | GLU | 294 | 37.070 | -36.040 | 15.905 | 1.00 | 0.00 | 3A7 |
| ATOM | 2022 | OE2 | GLU | 294 | 39.285 | -36.104 | 15.722 | 1.00 | 0.00 | 3A7 |
| ATOM | 2023 | C   | GLU | 294 | 36.901 | -31.676 | 18.723 | 1.00 | 0.00 | 3A7 |
| ATOM | 2024 | O   | GLU | 294 | 35.776 | -31.192 | 18.632 | 1.00 | 0.00 | 3A7 |
| ATOM | 2025 | N   | LEU | 295 | 37.506 | -31.876 | 19.909 | 1.00 | 0.00 | 3A7 |
| ATOM | 2026 | CA  | LEU | 295 | 36.915 | -31.573 | 21.190 | 1.00 | 0.00 | 3A7 |
| ATOM | 2027 | CB  | LEU | 295 | 37.911 | -31.878 | 22.313 | 1.00 | 0.00 | 3A7 |
| ATOM | 2028 | CG  | LEU | 295 | 38.311 | -33.358 | 22.435 | 1.00 | 0.00 | 3A7 |
| ATOM | 2029 | CD1 | LEU | 295 | 39.434 | -33.555 | 23.470 | 1.00 | 0.00 | 3A7 |
| ATOM | 2030 | CD2 | LEU | 295 | 37.094 | -34.206 | 22.783 | 1.00 | 0.00 | 3A7 |
| ATOM | 2031 | C   | LEU | 295 | 36.535 | -30.119 | 21.312 | 1.00 | 0.00 | 3A7 |
| ATOM | 2032 | O   | LEU | 295 | 35.404 | -29.765 | 21.643 | 1.00 | 0.00 | 3A7 |
| ATOM | 2033 | N   | MET | 296 | 37.488 | -29.212 | 21.017 | 1.00 | 0.00 | 3A7 |
| ATOM | 2034 | CA  | MET | 296 | 37.285 | -27.783 | 21.050 | 1.00 | 0.00 | 3A7 |
| ATOM | 2035 | CB  | MET | 296 | 38.580 | -27.070 | 20.647 | 1.00 | 0.00 | 3A7 |
| ATOM | 2036 | CG  | MET | 296 | 38.420 | -25.578 | 20.350 | 1.00 | 0.00 | 3A7 |
| ATOM | 2037 | SD  | MET | 296 | 40.016 | -24.717 | 20.404 | 1.00 | 0.00 | 3A7 |
| ATOM | 2038 | CE  | MET | 296 | 40.777 | -25.540 | 18.974 | 1.00 | 0.00 | 3A7 |
| ATOM | 2039 | C   | MET | 296 | 36.195 | -27.341 | 20.113 | 1.00 | 0.00 | 3A7 |
| ATOM | 2040 | O   | MET | 296 | 35.328 | -26.566 | 20.489 | 1.00 | 0.00 | 3A7 |
| ATOM | 2041 | N   | ALA | 297 | 36.174 | -27.882 | 18.877 | 1.00 | 0.00 | 3A7 |
| ATOM | 2042 | CA  | ALA | 297 | 35.172 | -27.555 | 17.895 | 1.00 | 0.00 | 3A7 |
| ATOM | 2043 | CB  | ALA | 297 | 35.493 | -28.182 | 16.525 | 1.00 | 0.00 | 3A7 |
| ATOM | 2044 | C   | ALA | 297 | 33.783 | -27.978 | 18.300 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2045 | O   | ALA | 297 | 32.817 | -27.301 | 17.986 | 1.00 | 0.00 | 3A7 |
| ATOM | 2046 | N   | GLN | 298 | 33.648 | -29.071 | 19.085 | 1.00 | 0.00 | 3A7 |
| ATOM | 2047 | CA  | GLN | 298 | 32.385 | -29.501 | 19.640 | 1.00 | 0.00 | 3A7 |
| ATOM | 2048 | CB  | GLN | 298 | 32.482 | -30.905 | 20.248 | 1.00 | 0.00 | 3A7 |
| ATOM | 2049 | CG  | GLN | 298 | 32.651 | -32.025 | 19.207 | 1.00 | 0.00 | 3A7 |
| ATOM | 2050 | CD  | GLN | 298 | 32.958 | -33.345 | 19.922 | 1.00 | 0.00 | 3A7 |
| ATOM | 2051 | OE1 | GLN | 298 | 34.080 | -33.554 | 20.400 | 1.00 | 0.00 | 3A7 |
| ATOM | 2052 | NE2 | GLN | 298 | 31.939 | -34.253 | 19.977 | 1.00 | 0.00 | 3A7 |
| ATOM | 2053 | C   | GLN | 298 | 31.922 | -28.563 | 20.719 | 1.00 | 0.00 | 3A7 |
| ATOM | 2054 | O   | GLN | 298 | 30.773 | -28.142 | 20.728 | 1.00 | 0.00 | 3A7 |
| ATOM | 2055 | N   | SER | 299 | 32.831 | -28.160 | 21.630 | 1.00 | 0.00 | 3A7 |
| ATOM | 2056 | CA  | SER | 299 | 32.535 | -27.222 | 22.690 | 1.00 | 0.00 | 3A7 |
| ATOM | 2057 | CB  | SER | 299 | 33.759 | -27.023 | 23.597 | 1.00 | 0.00 | 3A7 |
| ATOM | 2058 | OG  | SER | 299 | 34.175 | -28.269 | 24.141 | 1.00 | 0.00 | 3A7 |
| ATOM | 2059 | C   | SER | 299 | 32.097 | -25.874 | 22.158 | 1.00 | 0.00 | 3A7 |
| ATOM | 2060 | O   | SER | 299 | 31.185 | -25.252 | 22.698 | 1.00 | 0.00 | 3A7 |
| ATOM | 2061 | N   | ILE | 300 | 32.719 | -25.399 | 21.047 | 1.00 | 0.00 | 3A7 |
| ATOM | 2062 | CA  | ILE | 300 | 32.361 | -24.170 | 20.361 | 1.00 | 0.00 | 3A7 |
| ATOM | 2063 | CB  | ILE | 300 | 33.321 | -23.832 | 19.229 | 1.00 | 0.00 | 3A7 |
| ATOM | 2064 | CG2 | ILE | 300 | 32.843 | -22.603 | 18.412 | 1.00 | 0.00 | 3A7 |
| ATOM | 2065 | CG1 | ILE | 300 | 34.732 | -23.560 | 19.774 | 1.00 | 0.00 | 3A7 |
| ATOM | 2066 | CD  | ILE | 300 | 35.811 | -23.539 | 18.691 | 1.00 | 0.00 | 3A7 |
| ATOM | 2067 | C   | ILE | 300 | 30.987 | -24.293 | 19.764 | 1.00 | 0.00 | 3A7 |
| ATOM | 2068 | O   | ILE | 300 | 30.162 | -23.398 | 19.914 | 1.00 | 0.00 | 3A7 |
| ATOM | 2069 | N   | ILE | 301 | 30.695 | -25.431 | 19.092 | 1.00 | 0.00 | 3A7 |
| ATOM | 2070 | CA  | ILE | 301 | 29.418 | -25.676 | 18.455 | 1.00 | 0.00 | 3A7 |
| ATOM | 2071 | CB  | ILE | 301 | 29.475 | -26.900 | 17.553 | 1.00 | 0.00 | 3A7 |
| ATOM | 2072 | CG2 | ILE | 301 | 28.192 | -27.772 | 17.525 | 1.00 | 0.00 | 3A7 |
| ATOM | 2073 | CG1 | ILE | 301 | 29.774 | -26.460 | 16.091 | 1.00 | 0.00 | 3A7 |
| ATOM | 2074 | CD  | ILE | 301 | 31.053 | -25.647 | 15.869 | 1.00 | 0.00 | 3A7 |
| ATOM | 2075 | C   | ILE | 301 | 28.303 | -25.792 | 19.465 | 1.00 | 0.00 | 3A7 |
| ATOM | 2076 | O   | ILE | 301 | 27.182 | -25.379 | 19.205 | 1.00 | 0.00 | 3A7 |
| ATOM | 2077 | N   | PHE | 302 | 28.584 | -26.318 | 20.673 | 1.00 | 0.00 | 3A7 |
| ATOM | 2078 | CA  | PHE | 302 | 27.593 | -26.507 | 21.709 | 1.00 | 0.00 | 3A7 |
| ATOM | 2079 | CB  | PHE | 302 | 28.212 | -27.306 | 22.878 | 1.00 | 0.00 | 3A7 |
| ATOM | 2080 | CG  | PHE | 302 | 28.239 | -28.790 | 22.660 | 1.00 | 0.00 | 3A7 |
| ATOM | 2081 | CD1 | PHE | 302 | 28.348 | -29.335 | 21.379 | 1.00 | 0.00 | 3A7 |
| ATOM | 2082 | CD2 | PHE | 302 | 28.620 | -29.577 | 23.757 | 1.00 | 0.00 | 3A7 |
| ATOM | 2083 | CE1 | PHE | 302 | 28.914 | -30.584 | 21.188 | 1.00 | 0.00 | 3A7 |
| ATOM | 2084 | CE2 | PHE | 302 | 29.170 | -30.829 | 23.567 | 1.00 | 0.00 | 3A7 |
| ATOM | 2085 | CZ  | PHE | 302 | 29.356 | -31.311 | 22.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 2086 | C   | PHE | 302 | 27.161 | -25.150 | 22.252 | 1.00 | 0.00 | 3A7 |
| ATOM | 2087 | O   | PHE | 302 | 25.980 | -24.892 | 22.478 | 1.00 | 0.00 | 3A7 |
| ATOM | 2088 | N   | ILE | 303 | 28.134 | -24.221 | 22.452 | 1.00 | 0.00 | 3A7 |
| ATOM | 2089 | CA  | ILE | 303 | 27.866 | -22.889 | 22.966 | 1.00 | 0.00 | 3A7 |
| ATOM | 2090 | CB  | ILE | 303 | 29.091 | -22.188 | 23.539 | 1.00 | 0.00 | 3A7 |
| ATOM | 2091 | CG2 | ILE | 303 | 28.716 | -20.768 | 24.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 2092 | CG1 | ILE | 303 | 29.642 | -23.043 | 24.700 | 1.00 | 0.00 | 3A7 |
| ATOM | 2093 | CD  | ILE | 303 | 30.952 | -22.513 | 25.280 | 1.00 | 0.00 | 3A7 |
| ATOM | 2094 | C   | ILE | 303 | 27.215 | -22.030 | 21.914 | 1.00 | 0.00 | 3A7 |
| ATOM | 2095 | O   | ILE | 303 | 26.217 | -21.376 | 22.173 | 1.00 | 0.00 | 3A7 |
| ATOM | 2096 | N   | PHE | 304 | 27.728 | -22.042 | 20.671 | 1.00 | 0.00 | 3A7 |
| ATOM | 2097 | CA  | PHE | 304 | 27.197 | -21.301 | 19.548 | 1.00 | 0.00 | 3A7 |
| ATOM | 2098 | CB  | PHE | 304 | 28.117 | -21.579 | 18.314 | 1.00 | 0.00 | 3A7 |
| ATOM | 2099 | CG  | PHE | 304 | 27.669 | -20.996 | 16.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 2100 | CD1 | PHE | 304 | 27.839 | -19.644 | 16.704 | 1.00 | 0.00 | 3A7 |
| ATOM | 2101 | CD2 | PHE | 304 | 27.091 | -21.829 | 16.036 | 1.00 | 0.00 | 3A7 |
| ATOM | 2102 | CE1 | PHE | 304 | 27.436 | -19.134 | 15.472 | 1.00 | 0.00 | 3A7 |
| ATOM | 2103 | CE2 | PHE | 304 | 26.678 | -21.320 | 14.811 | 1.00 | 0.00 | 3A7 |
| ATOM | 2104 | CZ  | PHE | 304 | 26.851 | -19.970 | 14.526 | 1.00 | 0.00 | 3A7 |
| ATOM | 2105 | C   | PHE | 304 | 25.772 | -21.649 | 19.207 | 1.00 | 0.00 | 3A7 |
| ATOM | 2106 | O   | PHE | 304 | 24.909 | -20.780 | 19.129 | 1.00 | 0.00 | 3A7 |
| ATOM | 2107 | N   | ALA | 305 | 25.493 | -22.954 | 19.027 | 1.00 | 0.00 | 3A7 |
| ATOM | 2108 | CA  | ALA | 305 | 24.183 | -23.428 | 18.672 | 1.00 | 0.00 | 3A7 |
| ATOM | 2109 | CB  | ALA | 305 | 24.206 | -24.883 | 18.216 | 1.00 | 0.00 | 3A7 |
| ATOM | 2110 | C   | ALA | 305 | 23.224 | -23.354 | 19.820 | 1.00 | 0.00 | 3A7 |
| ATOM | 2111 | O   | ALA | 305 | 22.041 | -23.132 | 19.620 | 1.00 | 0.00 | 3A7 |
| ATOM | 2112 | N   | GLY | 306 | 23.734 | -23.533 | 21.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 2113 | CA  | GLY | 306 | 22.903 | -23.642 | 22.219 | 1.00 | 0.00 | 3A7 |
| ATOM | 2114 | C   | GLY | 306 | 22.541 | -22.346 | 22.888 | 1.00 | 0.00 | 3A7 |
| ATOM | 2115 | O   | GLY | 306 | 21.518 | -22.258 | 23.561 | 1.00 | 0.00 | 3A7 |
| ATOM | 2116 | N   | TYR | 307 | 23.359 | -21.285 | 22.742 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2117 | CA  | TYR | 307 | 23.134 | -20.054 | 23.474 | 1.00 | 0.00 | 3A7 |
| ATOM | 2118 | CB  | TYR | 307 | 24.473 | -19.279 | 23.690 | 1.00 | 0.00 | 3A7 |
| ATOM | 2119 | CG  | TYR | 307 | 24.492 | -17.764 | 23.545 | 1.00 | 0.00 | 3A7 |
| ATOM | 2120 | CD1 | TYR | 307 | 23.675 | -16.927 | 24.308 | 1.00 | 0.00 | 3A7 |
| ATOM | 2121 | CD2 | TYR | 307 | 25.364 | -17.182 | 22.621 | 1.00 | 0.00 | 3A7 |
| ATOM | 2122 | CE1 | TYR | 307 | 23.720 | -15.545 | 24.144 | 1.00 | 0.00 | 3A7 |
| ATOM | 2123 | CE2 | TYR | 307 | 25.420 | -15.801 | 22.460 | 1.00 | 0.00 | 3A7 |
| ATOM | 2124 | CZ  | TYR | 307 | 24.595 | -14.980 | 23.222 | 1.00 | 0.00 | 3A7 |
| ATOM | 2125 | OH  | TYR | 307 | 24.653 | -13.578 | 23.066 | 1.00 | 0.00 | 3A7 |
| ATOM | 2126 | C   | TYR | 307 | 22.056 | -19.224 | 22.841 | 1.00 | 0.00 | 3A7 |
| ATOM | 2127 | O   | TYR | 307 | 21.092 | -18.851 | 23.498 | 1.00 | 0.00 | 3A7 |
| ATOM | 2128 | N   | GLU | 308 | 22.222 | -18.888 | 21.552 | 1.00 | 0.00 | 3A7 |
| ATOM | 2129 | CA  | GLU | 308 | 21.442 | -17.887 | 20.875 | 1.00 | 0.00 | 3A7 |
| ATOM | 2130 | CB  | GLU | 308 | 22.048 | -17.593 | 19.488 | 1.00 | 0.00 | 3A7 |
| ATOM | 2131 | CG  | GLU | 308 | 22.280 | -18.862 | 18.631 | 1.00 | 0.00 | 3A7 |
| ATOM | 2132 | CD  | GLU | 308 | 23.057 | -18.569 | 17.347 | 1.00 | 0.00 | 3A7 |
| ATOM | 2133 | OE1 | GLU | 308 | 23.277 | -17.372 | 17.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 2134 | OE2 | GLU | 308 | 23.430 | -19.556 | 16.657 | 1.00 | 0.00 | 3A7 |
| ATOM | 2135 | C   | GLU | 308 | 20.007 | -18.253 | 20.661 | 1.00 | 0.00 | 3A7 |
| ATOM | 2136 | O   | GLU | 308 | 19.119 | -17.424 | 20.814 | 1.00 | 0.00 | 3A7 |
| ATOM | 2137 | N   | THR | 309 | 19.741 | -19.531 | 20.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 2138 | CA  | THR | 309 | 18.413 | -20.055 | 20.080 | 1.00 | 0.00 | 3A7 |
| ATOM | 2139 | CB  | THR | 309 | 18.504 | -21.431 | 19.437 | 1.00 | 0.00 | 3A7 |
| ATOM | 2140 | OG1 | THR | 309 | 17.244 | -21.870 | 18.974 | 1.00 | 0.00 | 3A7 |
| ATOM | 2141 | CG2 | THR | 309 | 19.256 | -22.438 | 20.330 | 1.00 | 0.00 | 3A7 |
| ATOM | 2142 | C   | THR | 309 | 17.592 | -20.080 | 21.350 | 1.00 | 0.00 | 3A7 |
| ATOM | 2143 | O   | THR | 309 | 16.436 | -19.681 | 21.350 | 1.00 | 0.00 | 3A7 |
| ATOM | 2144 | N   | THR | 310 | 18.187 | -20.515 | 22.480 | 1.00 | 0.00 | 3A7 |
| ATOM | 2145 | CA  | THR | 310 | 17.519 | -20.567 | 23.760 | 1.00 | 0.00 | 3A7 |
| ATOM | 2146 | CB  | THR | 310 | 18.271 | -21.435 | 24.744 | 1.00 | 0.00 | 3A7 |
| ATOM | 2147 | OG1 | THR | 310 | 18.739 | -22.609 | 24.101 | 1.00 | 0.00 | 3A7 |
| ATOM | 2148 | CG2 | THR | 310 | 17.383 | -21.832 | 25.943 | 1.00 | 0.00 | 3A7 |
| ATOM | 2149 | C   | THR | 310 | 17.233 | -19.209 | 24.344 | 1.00 | 0.00 | 3A7 |
| ATOM | 2150 | O   | THR | 310 | 16.168 | -18.987 | 24.914 | 1.00 | 0.00 | 3A7 |
| ATOM | 2151 | N   | SER | 311 | 18.147 | -18.228 | 24.167 | 1.00 | 0.00 | 3A7 |
| ATOM | 2152 | CA  | SER | 311 | 17.925 | -16.885 | 24.659 | 1.00 | 0.00 | 3A7 |
| ATOM | 2153 | CB  | SER | 311 | 19.171 | -15.993 | 24.620 | 1.00 | 0.00 | 3A7 |
| ATOM | 2154 | OG  | SER | 311 | 20.346 | -16.710 | 24.906 | 1.00 | 0.00 | 3A7 |
| ATOM | 2155 | C   | SER | 311 | 16.857 | -16.191 | 23.854 | 1.00 | 0.00 | 3A7 |
| ATOM | 2156 | O   | SER | 311 | 15.998 | -15.515 | 24.407 | 1.00 | 0.00 | 3A7 |
| ATOM | 2157 | N   | SER | 312 | 16.848 | -16.368 | 22.505 | 1.00 | 0.00 | 3A7 |
| ATOM | 2158 | CA  | SER | 312 | 15.858 | -15.769 | 21.625 | 1.00 | 0.00 | 3A7 |
| ATOM | 2159 | CB  | SER | 312 | 16.203 | -15.894 | 20.128 | 1.00 | 0.00 | 3A7 |
| ATOM | 2160 | OG  | SER | 312 | 16.398 | -17.244 | 19.751 | 1.00 | 0.00 | 3A7 |
| ATOM | 2161 | C   | SER | 312 | 14.473 | -16.334 | 21.903 | 1.00 | 0.00 | 3A7 |
| ATOM | 2162 | O   | SER | 312 | 13.477 | -15.641 | 21.718 | 1.00 | 0.00 | 3A7 |
| ATOM | 2163 | N   | VAL | 313 | 14.376 | -17.602 | 22.376 | 1.00 | 0.00 | 3A7 |
| ATOM | 2164 | CA  | VAL | 313 | 13.115 | -18.232 | 22.678 | 1.00 | 0.00 | 3A7 |
| ATOM | 2165 | CB  | VAL | 313 | 13.262 | -19.732 | 22.736 | 1.00 | 0.00 | 3A7 |
| ATOM | 2166 | CG1 | VAL | 313 | 12.003 | -20.440 | 23.260 | 1.00 | 0.00 | 3A7 |
| ATOM | 2167 | CG2 | VAL | 313 | 13.426 | -20.126 | 21.263 | 1.00 | 0.00 | 3A7 |
| ATOM | 2168 | C   | VAL | 313 | 12.555 | -17.712 | 23.971 | 1.00 | 0.00 | 3A7 |
| ATOM | 2169 | O   | VAL | 313 | 11.368 | -17.425 | 24.059 | 1.00 | 0.00 | 3A7 |
| ATOM | 2170 | N   | LEU | 314 | 13.406 | -17.522 | 25.000 | 1.00 | 0.00 | 3A7 |
| ATOM | 2171 | CA  | LEU | 314 | 13.003 | -16.991 | 26.283 | 1.00 | 0.00 | 3A7 |
| ATOM | 2172 | CB  | LEU | 314 | 14.178 | -17.030 | 27.279 | 1.00 | 0.00 | 3A7 |
| ATOM | 2173 | CG  | LEU | 314 | 14.712 | -18.444 | 27.608 | 1.00 | 0.00 | 3A7 |
| ATOM | 2174 | CD1 | LEU | 314 | 16.160 | -18.400 | 28.135 | 1.00 | 0.00 | 3A7 |
| ATOM | 2175 | CD2 | LEU | 314 | 13.817 | -19.188 | 28.604 | 1.00 | 0.00 | 3A7 |
| ATOM | 2176 | C   | LEU | 314 | 12.519 | -15.573 | 26.181 | 1.00 | 0.00 | 3A7 |
| ATOM | 2177 | O   | LEU | 314 | 11.490 | -15.204 | 26.736 | 1.00 | 0.00 | 3A7 |
| ATOM | 2178 | N   | SER | 315 | 13.252 | -14.741 | 25.411 | 1.00 | 0.00 | 3A7 |
| ATOM | 2179 | CA  | SER | 315 | 12.914 | -13.355 | 25.165 | 1.00 | 0.00 | 3A7 |
| ATOM | 2180 | CB  | SER | 315 | 14.033 | -12.603 | 24.406 | 1.00 | 0.00 | 3A7 |
| ATOM | 2181 | OG  | SER | 315 | 15.234 | -12.612 | 25.166 | 1.00 | 0.00 | 3A7 |
| ATOM | 2182 | C   | SER | 315 | 11.625 | -13.209 | 24.374 | 1.00 | 0.00 | 3A7 |
| ATOM | 2183 | O   | SER | 315 | 10.814 | -12.336 | 24.676 | 1.00 | 0.00 | 3A7 |
| ATOM | 2184 | N   | PHE | 316 | 11.391 | -14.075 | 23.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 2185 | CA  | PHE | 316 | 10.164 | -14.069 | 22.587 | 1.00 | 0.00 | 3A7 |
| ATOM | 2186 | CB  | PHE | 316 | 10.264 | -14.913 | 21.289 | 1.00 | 0.00 | 3A7 |
| ATOM | 2187 | CG  | PHE | 316 | 10.697 | -14.085 | 20.108 | 1.00 | 0.00 | 3A7 |
| ATOM | 2188 | CD1 | PHE | 316 | 11.810 | -14.439 | 19.342 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2189 | CD2 | PHE | 316 | 9.933  | -12.985 | 19.709 | 1.00 | 0.00 | 3A7 |
| ATOM | 2190 | CE1 | PHE | 316 | 12.165 | -13.699 | 18.217 | 1.00 | 0.00 | 3A7 |
| ATOM | 2191 | CE2 | PHE | 316 | 10.281 | -12.246 | 18.582 | 1.00 | 0.00 | 3A7 |
| ATOM | 2192 | CZ  | PHE | 316 | 11.402 | -12.600 | 17.837 | 1.00 | 0.00 | 3A7 |
| ATOM | 2193 | C   | PHE | 316 | 9.015  | -14.618 | 23.406 | 1.00 | 0.00 | 3A7 |
| ATOM | 2194 | O   | PHE | 316 | 7.891  | -14.133 | 23.296 | 1.00 | 0.00 | 3A7 |
| ATOM | 2195 | N   | ILE | 317 | 9.257  | -15.617 | 24.306 | 1.00 | 0.00 | 3A7 |
| ATOM | 2196 | CA  | ILE | 317 | 8.200  | -16.171 | 25.144 | 1.00 | 0.00 | 3A7 |
| ATOM | 2197 | CB  | ILE | 317 | 8.522  | -17.418 | 26.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 2198 | CG2 | ILE | 317 | 7.716  | -17.454 | 27.357 | 1.00 | 0.00 | 3A7 |
| ATOM | 2199 | CG1 | ILE | 317 | 8.150  | -18.749 | 25.331 | 1.00 | 0.00 | 3A7 |
| ATOM | 2200 | CD  | ILE | 317 | 9.210  | -19.340 | 24.419 | 1.00 | 0.00 | 3A7 |
| ATOM | 2201 | C   | ILE | 317 | 7.672  | -15.117 | 26.091 | 1.00 | 0.00 | 3A7 |
| ATOM | 2202 | O   | ILE | 317 | 6.464  | -14.997 | 26.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 2203 | N   | ILE | 318 | 8.566  | -14.313 | 26.715 | 1.00 | 0.00 | 3A7 |
| ATOM | 2204 | CA  | ILE | 318 | 8.192  | -13.252 | 27.635 | 1.00 | 0.00 | 3A7 |
| ATOM | 2205 | CB  | ILE | 318 | 9.425  | -12.624 | 28.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 2206 | CG2 | ILE | 318 | 9.076  | -11.357 | 29.092 | 1.00 | 0.00 | 3A7 |
| ATOM | 2207 | CG1 | ILE | 318 | 10.087 | -13.689 | 29.181 | 1.00 | 0.00 | 3A7 |
| ATOM | 2208 | CD  | ILE | 318 | 11.481 | -13.295 | 29.665 | 1.00 | 0.00 | 3A7 |
| ATOM | 2209 | C   | ILE | 318 | 7.339  | -12.213 | 26.942 | 1.00 | 0.00 | 3A7 |
| ATOM | 2210 | O   | ILE | 318 | 6.296  | -11.802 | 27.441 | 1.00 | 0.00 | 3A7 |
| ATOM | 2211 | N   | TYR | 319 | 7.731  | -11.823 | 25.716 | 1.00 | 0.00 | 3A7 |
| ATOM | 2212 | CA  | TYR | 319 | 6.987  | -10.893 | 24.906 | 1.00 | 0.00 | 3A7 |
| ATOM | 2213 | CB  | TYR | 319 | 7.729  | -10.658 | 23.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 2214 | CG  | TYR | 319 | 6.940  | -9.879  | 22.557 | 1.00 | 0.00 | 3A7 |
| ATOM | 2215 | CD1 | TYR | 319 | 6.414  | -8.628  | 22.863 | 1.00 | 0.00 | 3A7 |
| ATOM | 2216 | CD2 | TYR | 319 | 6.693  | -10.438 | 21.301 | 1.00 | 0.00 | 3A7 |
| ATOM | 2217 | CE1 | TYR | 319 | 5.597  | -7.976  | 21.949 | 1.00 | 0.00 | 3A7 |
| ATOM | 2218 | CE2 | TYR | 319 | 5.898  | -9.773  | 20.375 | 1.00 | 0.00 | 3A7 |
| ATOM | 2219 | CZ  | TYR | 319 | 5.336  | -8.544  | 20.704 | 1.00 | 0.00 | 3A7 |
| ATOM | 2220 | OH  | TYR | 319 | 4.491  | -7.887  | 19.783 | 1.00 | 0.00 | 3A7 |
| ATOM | 2221 | C   | TYR | 319 | 5.568  | -11.359 | 24.631 | 1.00 | 0.00 | 3A7 |
| ATOM | 2222 | O   | TYR | 319 | 4.622  | -10.588 | 24.752 | 1.00 | 0.00 | 3A7 |
| ATOM | 2223 | N   | GLU | 320 | 5.404  | -12.651 | 24.277 | 1.00 | 0.00 | 3A7 |
| ATOM | 2224 | CA  | GLU | 320 | 4.118  | -13.205 | 23.952 | 1.00 | 0.00 | 3A7 |
| ATOM | 2225 | CB  | GLU | 320 | 4.190  | -14.545 | 23.220 | 1.00 | 0.00 | 3A7 |
| ATOM | 2226 | CG  | GLU | 320 | 4.824  | -14.416 | 21.829 | 1.00 | 0.00 | 3A7 |
| ATOM | 2227 | CD  | GLU | 320 | 3.795  | -13.768 | 20.915 | 1.00 | 0.00 | 3A7 |
| ATOM | 2228 | OE1 | GLU | 320 | 4.068  | -12.634 | 20.435 | 1.00 | 0.00 | 3A7 |
| ATOM | 2229 | OE2 | GLU | 320 | 2.723  | -14.384 | 20.681 | 1.00 | 0.00 | 3A7 |
| ATOM | 2230 | C   | GLU | 320 | 3.209  | -13.345 | 25.140 | 1.00 | 0.00 | 3A7 |
| ATOM | 2231 | O   | GLU | 320 | 2.018  | -13.087 | 25.041 | 1.00 | 0.00 | 3A7 |
| ATOM | 2232 | N   | LEU | 321 | 3.746  | -13.705 | 26.321 | 1.00 | 0.00 | 3A7 |
| ATOM | 2233 | CA  | LEU | 321 | 2.972  | -13.799 | 27.537 | 1.00 | 0.00 | 3A7 |
| ATOM | 2234 | CB  | LEU | 321 | 3.805  | -14.427 | 28.662 | 1.00 | 0.00 | 3A7 |
| ATOM | 2235 | CG  | LEU | 321 | 4.011  | -15.941 | 28.472 | 1.00 | 0.00 | 3A7 |
| ATOM | 2236 | CD1 | LEU | 321 | 5.072  | -16.456 | 29.453 | 1.00 | 0.00 | 3A7 |
| ATOM | 2237 | CD2 | LEU | 321 | 2.687  | -16.706 | 28.641 | 1.00 | 0.00 | 3A7 |
| ATOM | 2238 | C   | LEU | 321 | 2.505  | -12.447 | 28.007 | 1.00 | 0.00 | 3A7 |
| ATOM | 2239 | O   | LEU | 321 | 1.395  | -12.302 | 28.509 | 1.00 | 0.00 | 3A7 |
| ATOM | 2240 | N   | ALA | 322 | 3.360  | -11.421 | 27.837 | 1.00 | 0.00 | 3A7 |
| ATOM | 2241 | CA  | ALA | 322 | 3.065  | -10.068 | 28.220 | 1.00 | 0.00 | 3A7 |
| ATOM | 2242 | CB  | ALA | 322 | 4.351  | -9.229  | 28.225 | 1.00 | 0.00 | 3A7 |
| ATOM | 2243 | C   | ALA | 322 | 2.044  | -9.469  | 27.279 | 1.00 | 0.00 | 3A7 |
| ATOM | 2244 | O   | ALA | 322 | 1.166  | -8.702  | 27.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 2245 | N   | THR | 323 | 2.110  | -9.863  | 25.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 2246 | CA  | THR | 323 | 1.174  | -9.402  | 25.006 | 1.00 | 0.00 | 3A7 |
| ATOM | 2247 | CB  | THR | 323 | 1.714  | -9.509  | 23.612 | 1.00 | 0.00 | 3A7 |
| ATOM | 2248 | OG1 | THR | 323 | 2.224  | -10.786 | 23.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 2249 | CG2 | THR | 323 | 2.782  | -8.417  | 23.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 2250 | C   | THR | 323 | -0.164 | -10.105 | 25.063 | 1.00 | 0.00 | 3A7 |
| ATOM | 2251 | O   | THR | 323 | -1.132 | -9.627  | 24.486 | 1.00 | 0.00 | 3A7 |
| ATOM | 2252 | N   | HIS | 324 | -0.258 | -11.241 | 25.774 | 1.00 | 0.00 | 3A7 |
| ATOM | 2253 | CA  | HIS | 324 | -1.475 | -12.018 | 25.882 | 1.00 | 0.00 | 3A7 |
| ATOM | 2254 | ND1 | HIS | 324 | -2.250 | -12.554 | 22.767 | 1.00 | 0.00 | 3A7 |
| ATOM | 2255 | CG  | HIS | 324 | -1.279 | -13.139 | 23.576 | 1.00 | 0.00 | 3A7 |
| ATOM | 2256 | CB  | HIS | 324 | -1.248 | -13.311 | 25.087 | 1.00 | 0.00 | 3A7 |
| ATOM | 2257 | NE2 | HIS | 324 | -0.359 | -12.447 | 21.617 | 1.00 | 0.00 | 3A7 |
| ATOM | 2258 | CD2 | HIS | 324 | -0.126 | -13.016 | 22.856 | 1.00 | 0.00 | 3A7 |
| ATOM | 2259 | CE1 | HIS | 324 | -1.648 | -12.187 | 21.610 | 1.00 | 0.00 | 3A7 |
| ATOM | 2260 | C   | HIS | 324 | -1.699 | -12.327 | 27.334 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2261 | O   | HIS | 324 | -1.410 | -13.448 | 27.764 | 1.00 | 0.00 | 3A7 |
| ATOM | 2262 | N   | PRO | 325 | -2.246 | -11.398 | 28.139 | 1.00 | 0.00 | 3A7 |
| ATOM | 2263 | CA  | PRO | 325 | -2.362 | -11.530 | 29.587 | 1.00 | 0.00 | 3A7 |
| ATOM | 2264 | CD  | PRO | 325 | -2.664 | -10.073 | 27.697 | 1.00 | 0.00 | 3A7 |
| ATOM | 2265 | CB  | PRO | 325 | -3.005 | -10.217 | 30.049 | 1.00 | 0.00 | 3A7 |
| ATOM | 2266 | CG  | PRO | 325 | -2.634 | -9.212  | 28.959 | 1.00 | 0.00 | 3A7 |
| ATOM | 2267 | C   | PRO | 325 | -3.219 | -12.703 | 30.001 | 1.00 | 0.00 | 3A7 |
| ATOM | 2268 | O   | PRO | 325 | -2.994 | -13.255 | 31.072 | 1.00 | 0.00 | 3A7 |
| ATOM | 2269 | N   | ASP | 326 | -4.183 | -13.144 | 29.162 | 1.00 | 0.00 | 3A7 |
| ATOM | 2270 | CA  | ASP | 326 | -5.016 | -14.290 | 29.448 | 1.00 | 0.00 | 3A7 |
| ATOM | 2271 | CB  | ASP | 326 | -6.108 | -14.480 | 28.372 | 1.00 | 0.00 | 3A7 |
| ATOM | 2272 | CG  | ASP | 326 | -7.091 | -13.305 | 28.363 | 1.00 | 0.00 | 3A7 |
| ATOM | 2273 | OD1 | ASP | 326 | -7.016 | -12.435 | 29.271 | 1.00 | 0.00 | 3A7 |
| ATOM | 2274 | OD2 | ASP | 326 | -7.946 | -13.276 | 27.437 | 1.00 | 0.00 | 3A7 |
| ATOM | 2275 | C   | ASP | 326 | -4.191 | -15.557 | 29.518 | 1.00 | 0.00 | 3A7 |
| ATOM | 2276 | O   | ASP | 326 | -4.391 | -16.408 | 30.379 | 1.00 | 0.00 | 3A7 |
| ATOM | 2277 | N   | VAL | 327 | -3.192 | -15.680 | 28.617 | 1.00 | 0.00 | 3A7 |
| ATOM | 2278 | CA  | VAL | 327 | -2.308 | -16.822 | 28.551 | 1.00 | 0.00 | 3A7 |
| ATOM | 2279 | CB  | VAL | 327 | -1.522 | -16.855 | 27.249 | 1.00 | 0.00 | 3A7 |
| ATOM | 2280 | CG1 | VAL | 327 | -0.634 | -18.114 | 27.189 | 1.00 | 0.00 | 3A7 |
| ATOM | 2281 | CG2 | VAL | 327 | -2.526 | -16.830 | 26.078 | 1.00 | 0.00 | 3A7 |
| ATOM | 2282 | C   | VAL | 327 | -1.357 | -16.811 | 29.718 | 1.00 | 0.00 | 3A7 |
| ATOM | 2283 | O   | VAL | 327 | -1.126 | -17.833 | 30.353 | 1.00 | 0.00 | 3A7 |
| ATOM | 2284 | N   | GLN | 328 | -0.822 | -15.622 | 30.057 | 1.00 | 0.00 | 3A7 |
| ATOM | 2285 | CA  | GLN | 328 | 0.054  | -15.440 | 31.190 | 1.00 | 0.00 | 3A7 |
| ATOM | 2286 | CB  | GLN | 328 | 0.551  | -13.994 | 31.280 | 1.00 | 0.00 | 3A7 |
| ATOM | 2287 | CG  | GLN | 328 | 1.927  | -13.874 | 31.956 | 1.00 | 0.00 | 3A7 |
| ATOM | 2288 | CD  | GLN | 328 | 2.430  | -12.432 | 31.850 | 1.00 | 0.00 | 3A7 |
| ATOM | 2289 | OE1 | GLN | 328 | 1.677  | -11.512 | 31.507 | 1.00 | 0.00 | 3A7 |
| ATOM | 2290 | NE2 | GLN | 328 | 3.749  | -12.247 | 32.162 | 1.00 | 0.00 | 3A7 |
| ATOM | 2291 | C   | GLN | 328 | -0.565 | -15.809 | 32.500 | 1.00 | 0.00 | 3A7 |
| ATOM | 2292 | O   | GLN | 328 | 0.057  | -16.448 | 33.339 | 1.00 | 0.00 | 3A7 |
| ATOM | 2293 | N   | GLN | 329 | -1.847 | -15.438 | 32.692 | 1.00 | 0.00 | 3A7 |
| ATOM | 2294 | CA  | GLN | 329 | -2.599 | -15.749 | 33.879 | 1.00 | 0.00 | 3A7 |
| ATOM | 2295 | CB  | GLN | 329 | -3.961 | -15.032 | 33.870 | 1.00 | 0.00 | 3A7 |
| ATOM | 2296 | CG  | GLN | 329 | -3.832 | -13.525 | 34.148 | 1.00 | 0.00 | 3A7 |
| ATOM | 2297 | CD  | GLN | 329 | -5.215 | -12.882 | 34.023 | 1.00 | 0.00 | 3A7 |
| ATOM | 2298 | OE1 | GLN | 329 | -6.121 | -13.175 | 34.813 | 1.00 | 0.00 | 3A7 |
| ATOM | 2299 | NE2 | GLN | 329 | -5.369 | -11.987 | 33.000 | 1.00 | 0.00 | 3A7 |
| ATOM | 2300 | C   | GLN | 329 | -2.821 | -17.226 | 34.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 2301 | O   | GLN | 329 | -2.653 | -17.780 | 35.102 | 1.00 | 0.00 | 3A7 |
| ATOM | 2302 | N   | LYS | 330 | -3.153 | -17.913 | 32.907 | 1.00 | 0.00 | 3A7 |
| ATOM | 2303 | CA  | LYS | 330 | -3.370 | -19.343 | 32.883 | 1.00 | 0.00 | 3A7 |
| ATOM | 2304 | CB  | LYS | 330 | -3.917 | -19.754 | 31.503 | 1.00 | 0.00 | 3A7 |
| ATOM | 2305 | CG  | LYS | 330 | -4.508 | -21.169 | 31.446 | 1.00 | 0.00 | 3A7 |
| ATOM | 2306 | CD  | LYS | 330 | -5.246 | -21.428 | 30.124 | 1.00 | 0.00 | 3A7 |
| ATOM | 2307 | CE  | LYS | 330 | -5.927 | -22.799 | 30.054 | 1.00 | 0.00 | 3A7 |
| ATOM | 2308 | NZ  | LYS | 330 | -6.952 | -22.943 | 31.113 | 1.00 | 0.00 | 3A7 |
| ATOM | 2309 | C   | LYS | 330 | -2.097 | -20.090 | 33.241 | 1.00 | 0.00 | 3A7 |
| ATOM | 2310 | O   | LYS | 330 | -2.090 | -21.027 | 34.040 | 1.00 | 0.00 | 3A7 |
| ATOM | 2311 | N   | VAL | 331 | -0.946 | -19.618 | 32.704 | 1.00 | 0.00 | 3A7 |
| ATOM | 2312 | CA  | VAL | 331 | 0.363  | -20.189 | 32.957 | 1.00 | 0.00 | 3A7 |
| ATOM | 2313 | CB  | VAL | 331 | 1.419  | -19.605 | 32.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 2314 | CG1 | VAL | 331 | 2.843  | -20.076 | 32.382 | 1.00 | 0.00 | 3A7 |
| ATOM | 2315 | CG2 | VAL | 331 | 1.080  | -20.072 | 30.601 | 1.00 | 0.00 | 3A7 |
| ATOM | 2316 | C   | VAL | 331 | 0.782  | -19.992 | 34.390 | 1.00 | 0.00 | 3A7 |
| ATOM | 2317 | O   | VAL | 331 | 1.274  | -20.919 | 35.023 | 1.00 | 0.00 | 3A7 |
| ATOM | 2318 | N   | GLN | 332 | 0.561  | -18.783 | 34.951 | 1.00 | 0.00 | 3A7 |
| ATOM | 2319 | CA  | GLN | 332 | 0.896  | -18.455 | 36.319 | 1.00 | 0.00 | 3A7 |
| ATOM | 2320 | CB  | GLN | 332 | 0.668  | -16.968 | 36.628 | 1.00 | 0.00 | 3A7 |
| ATOM | 2321 | CG  | GLN | 332 | 1.756  | -16.072 | 36.011 | 1.00 | 0.00 | 3A7 |
| ATOM | 2322 | CD  | GLN | 332 | 1.457  | -14.601 | 36.311 | 1.00 | 0.00 | 3A7 |
| ATOM | 2323 | OE1 | GLN | 332 | 2.196  | -13.947 | 37.057 | 1.00 | 0.00 | 3A7 |
| ATOM | 2324 | NE2 | GLN | 332 | 0.350  | -14.079 | 35.701 | 1.00 | 0.00 | 3A7 |
| ATOM | 2325 | C   | GLN | 332 | 0.082  | -19.234 | 37.311 | 1.00 | 0.00 | 3A7 |
| ATOM | 2326 | O   | GLN | 332 | 0.592  | -19.634 | 38.351 | 1.00 | 0.00 | 3A7 |
| ATOM | 2327 | N   | LYS | 333 | -1.200 | -19.512 | 36.991 | 1.00 | 0.00 | 3A7 |
| ATOM | 2328 | CA  | LYS | 333 | -2.087 | -20.320 | 37.797 | 1.00 | 0.00 | 3A7 |
| ATOM | 2329 | CB  | LYS | 333 | -3.508 | -20.312 | 37.204 | 1.00 | 0.00 | 3A7 |
| ATOM | 2330 | CG  | LYS | 333 | -4.571 | -21.052 | 38.035 | 1.00 | 0.00 | 3A7 |
| ATOM | 2331 | CD  | LYS | 333 | -5.986 | -20.945 | 37.441 | 1.00 | 0.00 | 3A7 |
| ATOM | 2332 | CE  | LYS | 333 | -6.125 | -21.617 | 36.068 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2333 | NZ  | LYS | 333 | -7.518 | -21.516 | 35.576 | 1.00 | 0.00 | 3A7 |
| ATOM | 2334 | C   | LYS | 333 | -1.600 | -21.746 | 37.882 | 1.00 | 0.00 | 3A7 |
| ATOM | 2335 | O   | LYS | 333 | -1.547 | -22.344 | 38.954 | 1.00 | 0.00 | 3A7 |
| ATOM | 2336 | N   | GLU | 334 | -1.171 | -22.295 | 36.728 | 1.00 | 0.00 | 3A7 |
| ATOM | 2337 | CA  | GLU | 334 | -0.533 | -23.579 | 36.649 | 1.00 | 0.00 | 3A7 |
| ATOM | 2338 | CB  | GLU | 334 | -0.149 | -23.952 | 35.224 | 1.00 | 0.00 | 3A7 |
| ATOM | 2339 | CG  | GLU | 334 | -0.038 | -25.481 | 35.122 | 1.00 | 0.00 | 3A7 |
| ATOM | 2340 | CD  | GLU | 334 | 0.087  | -25.922 | 33.672 | 1.00 | 0.00 | 3A7 |
| ATOM | 2341 | OE1 | GLU | 334 | -0.736 | -26.779 | 33.251 | 1.00 | 0.00 | 3A7 |
| ATOM | 2342 | OE2 | GLU | 334 | 1.007  | -25.424 | 32.971 | 1.00 | 0.00 | 3A7 |
| ATOM | 2343 | C   | GLU | 334 | 0.701  | -23.722 | 37.472 | 1.00 | 0.00 | 3A7 |
| ATOM | 2344 | O   | GLU | 334 | 0.825  | -24.667 | 38.236 | 1.00 | 0.00 | 3A7 |
| ATOM | 2345 | N   | ILE | 335 | 1.627  | -22.744 | 37.370 | 1.00 | 0.00 | 3A7 |
| ATOM | 2346 | CA  | ILE | 335 | 2.874  | -22.692 | 38.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 2347 | CB  | ILE | 335 | 3.672  | -21.474 | 37.679 | 1.00 | 0.00 | 3A7 |
| ATOM | 2348 | CG2 | ILE | 335 | 4.884  | -21.230 | 38.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 2349 | CG1 | ILE | 335 | 4.128  | -21.660 | 36.215 | 1.00 | 0.00 | 3A7 |
| ATOM | 2350 | CD  | ILE | 335 | 4.634  | -20.360 | 35.597 | 1.00 | 0.00 | 3A7 |
| ATOM | 2351 | C   | ILE | 335 | 2.643  | -22.684 | 39.587 | 1.00 | 0.00 | 3A7 |
| ATOM | 2352 | O   | ILE | 335 | 3.219  | -23.480 | 40.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 2353 | N   | ASP | 336 | 1.727  | -21.822 | 40.071 | 1.00 | 0.00 | 3A7 |
| ATOM | 2354 | CA  | ASP | 336 | 1.416  | -21.706 | 41.476 | 1.00 | 0.00 | 3A7 |
| ATOM | 2355 | CB  | ASP | 336 | 0.411  | -20.565 | 41.750 | 1.00 | 0.00 | 3A7 |
| ATOM | 2356 | CG  | ASP | 336 | 1.021  | -19.199 | 41.420 | 1.00 | 0.00 | 3A7 |
| ATOM | 2357 | OD1 | ASP | 336 | 2.243  | -19.127 | 41.123 | 1.00 | 0.00 | 3A7 |
| ATOM | 2358 | OD2 | ASP | 336 | 0.255  | -18.199 | 41.470 | 1.00 | 0.00 | 3A7 |
| ATOM | 2359 | C   | ASP | 336 | 0.838  | -22.996 | 42.010 | 1.00 | 0.00 | 3A7 |
| ATOM | 2360 | O   | ASP | 336 | 1.183  | -23.420 | 43.106 | 1.00 | 0.00 | 3A7 |
| ATOM | 2361 | N   | THR | 337 | -0.022 | -23.674 | 41.213 | 1.00 | 0.00 | 3A7 |
| ATOM | 2362 | CA  | THR | 337 | -0.701 | -24.903 | 41.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 2363 | CB  | THR | 337 | -1.854 | -25.156 | 40.609 | 1.00 | 0.00 | 3A7 |
| ATOM | 2364 | OG1 | THR | 337 | -2.791 | -24.092 | 40.721 | 1.00 | 0.00 | 3A7 |
| ATOM | 2365 | CG2 | THR | 337 | -2.601 | -26.473 | 40.896 | 1.00 | 0.00 | 3A7 |
| ATOM | 2366 | C   | THR | 337 | 0.216  | -26.114 | 41.595 | 1.00 | 0.00 | 3A7 |
| ATOM | 2367 | O   | THR | 337 | 0.055  | -27.000 | 42.433 | 1.00 | 0.00 | 3A7 |
| ATOM | 2368 | N   | VAL | 338 | 1.202  | -26.189 | 40.667 | 1.00 | 0.00 | 3A7 |
| ATOM | 2369 | CA  | VAL | 338 | 2.055  | -27.349 | 40.503 | 1.00 | 0.00 | 3A7 |
| ATOM | 2370 | CB  | VAL | 338 | 2.466  | -27.564 | 39.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 2371 | CG1 | VAL | 338 | 3.403  | -28.783 | 38.900 | 1.00 | 0.00 | 3A7 |
| ATOM | 2372 | CG2 | VAL | 338 | 1.182  | -27.789 | 38.226 | 1.00 | 0.00 | 3A7 |
| ATOM | 2373 | C   | VAL | 338 | 3.261  | -27.232 | 41.404 | 1.00 | 0.00 | 3A7 |
| ATOM | 2374 | O   | VAL | 338 | 3.589  | -28.178 | 42.113 | 1.00 | 0.00 | 3A7 |
| ATOM | 2375 | N   | LEU | 339 | 3.950  | -26.065 | 41.421 | 1.00 | 0.00 | 3A7 |
| ATOM | 2376 | CA  | LEU | 339 | 5.053  | -25.835 | 42.331 | 1.00 | 0.00 | 3A7 |
| ATOM | 2377 | CB  | LEU | 339 | 6.213  | -25.014 | 41.736 | 1.00 | 0.00 | 3A7 |
| ATOM | 2378 | CG  | LEU | 339 | 7.082  | -25.819 | 40.766 | 1.00 | 0.00 | 3A7 |
| ATOM | 2379 | CD1 | LEU | 339 | 8.159  | -24.904 | 40.176 | 1.00 | 0.00 | 3A7 |
| ATOM | 2380 | CD2 | LEU | 339 | 7.715  | -27.051 | 41.439 | 1.00 | 0.00 | 3A7 |
| ATOM | 2381 | C   | LEU | 339 | 4.552  | -25.038 | 43.521 | 1.00 | 0.00 | 3A7 |
| ATOM | 2382 | O   | LEU | 339 | 4.197  | -23.878 | 43.325 | 1.00 | 0.00 | 3A7 |
| ATOM | 2383 | N   | PRO | 340 | 4.486  | -25.565 | 44.752 | 1.00 | 0.00 | 3A7 |
| ATOM | 2384 | CA  | PRO | 340 | 3.973  | -24.851 | 45.907 | 1.00 | 0.00 | 3A7 |
| ATOM | 2385 | CD  | PRO | 340 | 4.660  | -26.986 | 45.025 | 1.00 | 0.00 | 3A7 |
| ATOM | 2386 | CB  | PRO | 340 | 3.483  | -25.968 | 46.840 | 1.00 | 0.00 | 3A7 |
| ATOM | 2387 | CG  | PRO | 340 | 4.398  | -27.154 | 46.523 | 1.00 | 0.00 | 3A7 |
| ATOM | 2388 | C   | PRO | 340 | 5.084  | -24.042 | 46.550 | 1.00 | 0.00 | 3A7 |
| ATOM | 2389 | O   | PRO | 340 | 6.241  | -24.463 | 46.512 | 1.00 | 0.00 | 3A7 |
| ATOM | 2390 | N   | ASN | 341 | 4.716  | -22.893 | 47.182 | 1.00 | 0.00 | 3A7 |
| ATOM | 2391 | CA  | ASN | 341 | 5.537  | -22.073 | 48.065 | 1.00 | 0.00 | 3A7 |
| ATOM | 2392 | CB  | ASN | 341 | 6.167  | -22.872 | 49.244 | 1.00 | 0.00 | 3A7 |
| ATOM | 2393 | CG  | ASN | 341 | 5.072  | -23.614 | 50.023 | 1.00 | 0.00 | 3A7 |
| ATOM | 2394 | OD1 | ASN | 341 | 5.051  | -24.850 | 50.059 | 1.00 | 0.00 | 3A7 |
| ATOM | 2395 | ND2 | ASN | 341 | 4.155  | -22.826 | 50.663 | 1.00 | 0.00 | 3A7 |
| ATOM | 2396 | C   | ASN | 341 | 6.625  | -21.330 | 47.312 | 1.00 | 0.00 | 3A7 |
| ATOM | 2397 | O   | ASN | 341 | 6.423  | -20.897 | 46.178 | 1.00 | 0.00 | 3A7 |
| ATOM | 2398 | N   | LYS | 342 | 7.813  | -21.175 | 47.953 | 1.00 | 0.00 | 3A7 |
| ATOM | 2399 | CA  | LYS | 342 | 8.980  | -20.529 | 47.396 | 1.00 | 0.00 | 3A7 |
| ATOM | 2400 | CB  | LYS | 342 | 9.578  | -19.456 | 48.339 | 1.00 | 0.00 | 3A7 |
| ATOM | 2401 | CG  | LYS | 342 | 8.601  | -18.309 | 48.647 | 1.00 | 0.00 | 3A7 |
| ATOM | 2402 | CD  | LYS | 342 | 9.210  | -17.205 | 49.527 | 1.00 | 0.00 | 3A7 |
| ATOM | 2403 | CE  | LYS | 342 | 9.570  | -17.674 | 50.944 | 1.00 | 0.00 | 3A7 |
| ATOM | 2404 | NZ  | LYS | 342 | 10.133 | -16.560 | 51.741 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2405 | C   | LYS | 342 | 10.016 | -21.594 | 47.146 | 1.00 | 0.00 | 3A7 |
| ATOM | 2406 | O   | LYS | 342 | 11.181 | -21.442 | 47.515 | 1.00 | 0.00 | 3A7 |
| ATOM | 2407 | N   | ALA | 343 | 9.595  | -22.711 | 46.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 2408 | CA  | ALA | 343 | 10.434 | -23.839 | 46.171 | 1.00 | 0.00 | 3A7 |
| ATOM | 2409 | CB  | ALA | 343 | 9.750  | -25.189 | 46.468 | 1.00 | 0.00 | 3A7 |
| ATOM | 2410 | C   | ALA | 343 | 10.737 | -23.763 | 44.700 | 1.00 | 0.00 | 3A7 |
| ATOM | 2411 | O   | ALA | 343 | 9.824  | -23.520 | 43.911 | 1.00 | 0.00 | 3A7 |
| ATOM | 2412 | N   | PRO | 344 | 11.980 | -24.000 | 44.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 2413 | CA  | PRO | 344 | 12.353 | -24.110 | 42.875 | 1.00 | 0.00 | 3A7 |
| ATOM | 2414 | CD  | PRO | 344 | 13.149 | -23.771 | 45.118 | 1.00 | 0.00 | 3A7 |
| ATOM | 2415 | CB  | PRO | 344 | 13.894 | -24.072 | 42.880 | 1.00 | 0.00 | 3A7 |
| ATOM | 2416 | CG  | PRO | 344 | 14.248 | -23.318 | 44.160 | 1.00 | 0.00 | 3A7 |
| ATOM | 2417 | C   | PRO | 344 | 11.838 | -25.414 | 42.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 2418 | O   | PRO | 344 | 11.420 | -26.289 | 43.033 | 1.00 | 0.00 | 3A7 |
| ATOM | 2419 | N   | PRO | 345 | 11.880 | -25.589 | 40.953 | 1.00 | 0.00 | 3A7 |
| ATOM | 2420 | CA  | PRO | 345 | 11.325 | -26.737 | 40.270 | 1.00 | 0.00 | 3A7 |
| ATOM | 2421 | CD  | PRO | 345 | 12.098 | -24.479 | 40.043 | 1.00 | 0.00 | 3A7 |
| ATOM | 2422 | CB  | PRO | 345 | 11.402 | -26.382 | 38.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 2423 | CG  | PRO | 345 | 11.412 | -24.857 | 38.731 | 1.00 | 0.00 | 3A7 |
| ATOM | 2424 | C   | PRO | 345 | 12.117 | -27.996 | 40.521 | 1.00 | 0.00 | 3A7 |
| ATOM | 2425 | O   | PRO | 345 | 13.329 | -27.934 | 40.723 | 1.00 | 0.00 | 3A7 |
| ATOM | 2426 | N   | THR | 346 | 11.432 | -29.156 | 40.428 | 1.00 | 0.00 | 3A7 |
| ATOM | 2427 | CA  | THR | 346 | 12.073 | -30.434 | 40.286 | 1.00 | 0.00 | 3A7 |
| ATOM | 2428 | CB  | THR | 346 | 11.485 | -31.522 | 41.180 | 1.00 | 0.00 | 3A7 |
| ATOM | 2429 | OG1 | THR | 346 | 10.071 | -31.633 | 41.047 | 1.00 | 0.00 | 3A7 |
| ATOM | 2430 | CG2 | THR | 346 | 11.830 | -31.183 | 42.644 | 1.00 | 0.00 | 3A7 |
| ATOM | 2431 | C   | THR | 346 | 11.920 | -30.751 | 38.827 | 1.00 | 0.00 | 3A7 |
| ATOM | 2432 | O   | THR | 346 | 11.346 | -29.983 | 38.054 | 1.00 | 0.00 | 3A7 |
| ATOM | 2433 | N   | TYR | 347 | 12.422 | -31.922 | 38.405 | 1.00 | 0.00 | 3A7 |
| ATOM | 2434 | CA  | TYR | 347 | 12.345 | -32.298 | 37.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 2435 | CB  | TYR | 347 | 13.345 | -33.383 | 36.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 2436 | CG  | TYR | 347 | 13.830 | -34.221 | 37.758 | 1.00 | 0.00 | 3A7 |
| ATOM | 2437 | CD1 | TYR | 347 | 13.226 | -35.455 | 38.007 | 1.00 | 0.00 | 3A7 |
| ATOM | 2438 | CD2 | TYR | 347 | 14.880 | -33.809 | 38.584 | 1.00 | 0.00 | 3A7 |
| ATOM | 2439 | CE1 | TYR | 347 | 13.653 | -36.258 | 39.060 | 1.00 | 0.00 | 3A7 |
| ATOM | 2440 | CE2 | TYR | 347 | 15.310 | -34.609 | 39.638 | 1.00 | 0.00 | 3A7 |
| ATOM | 2441 | CZ  | TYR | 347 | 14.697 | -35.835 | 39.877 | 1.00 | 0.00 | 3A7 |
| ATOM | 2442 | OH  | TYR | 347 | 15.133 | -36.649 | 40.945 | 1.00 | 0.00 | 3A7 |
| ATOM | 2443 | C   | TYR | 347 | 10.986 | -32.842 | 36.741 | 1.00 | 0.00 | 3A7 |
| ATOM | 2444 | O   | TYR | 347 | 10.471 | -32.653 | 35.655 | 1.00 | 0.00 | 3A7 |
| ATOM | 2445 | N   | ASP | 348 | 10.354 | -33.487 | 37.746 | 1.00 | 0.00 | 3A7 |
| ATOM | 2446 | CA  | ASP | 348 | 9.033  | -34.072 | 37.677 | 1.00 | 0.00 | 3A7 |
| ATOM | 2447 | CB  | ASP | 348 | 8.708  | -34.785 | 38.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 2448 | CG  | ASP | 348 | 9.678  | -35.950 | 39.163 | 1.00 | 0.00 | 3A7 |
| ATOM | 2449 | OD1 | ASP | 348 | 9.665  | -36.846 | 38.277 | 1.00 | 0.00 | 3A7 |
| ATOM | 2450 | OD2 | ASP | 348 | 10.439 | -35.959 | 40.167 | 1.00 | 0.00 | 3A7 |
| ATOM | 2451 | C   | ASP | 348 | 7.939  | -33.064 | 37.424 | 1.00 | 0.00 | 3A7 |
| ATOM | 2452 | O   | ASP | 348 | 6.884  | -33.393 | 36.890 | 1.00 | 0.00 | 3A7 |
| ATOM | 2453 | N   | THR | 349 | 8.224  | -31.784 | 37.764 | 1.00 | 0.00 | 3A7 |
| ATOM | 2454 | CA  | THR | 349 | 7.414  | -30.615 | 37.512 | 1.00 | 0.00 | 3A7 |
| ATOM | 2455 | CB  | THR | 349 | 8.047  | -29.394 | 38.153 | 1.00 | 0.00 | 3A7 |
| ATOM | 2456 | OG1 | THR | 349 | 8.345  | -29.682 | 39.512 | 1.00 | 0.00 | 3A7 |
| ATOM | 2457 | CG2 | THR | 349 | 7.118  | -28.168 | 38.103 | 1.00 | 0.00 | 3A7 |
| ATOM | 2458 | C   | THR | 349 | 7.246  | -30.355 | 36.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 2459 | O   | THR | 349 | 6.224  | -29.855 | 35.582 | 1.00 | 0.00 | 3A7 |
| ATOM | 2460 | N   | VAL | 350 | 8.243  | -30.735 | 35.203 | 1.00 | 0.00 | 3A7 |
| ATOM | 2461 | CA  | VAL | 350 | 8.261  | -30.585 | 33.760 | 1.00 | 0.00 | 3A7 |
| ATOM | 2462 | CB  | VAL | 350 | 9.589  | -31.111 | 33.245 | 1.00 | 0.00 | 3A7 |
| ATOM | 2463 | CG1 | VAL | 350 | 9.700  | -31.257 | 31.710 | 1.00 | 0.00 | 3A7 |
| ATOM | 2464 | CG2 | VAL | 350 | 10.704 | -30.188 | 33.784 | 1.00 | 0.00 | 3A7 |
| ATOM | 2465 | C   | VAL | 350 | 7.128  | -31.305 | 33.054 | 1.00 | 0.00 | 3A7 |
| ATOM | 2466 | O   | VAL | 350 | 6.691  | -30.900 | 31.980 | 1.00 | 0.00 | 3A7 |
| ATOM | 2467 | N   | LEU | 351 | 6.619  | -32.397 | 33.667 | 1.00 | 0.00 | 3A7 |
| ATOM | 2468 | CA  | LEU | 351 | 5.583  | -33.220 | 33.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 2469 | CB  | LEU | 351 | 5.689  | -34.682 | 33.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 2470 | CG  | LEU | 351 | 7.076  | -35.324 | 33.359 | 1.00 | 0.00 | 3A7 |
| ATOM | 2471 | CD1 | LEU | 351 | 7.162  | -36.712 | 34.024 | 1.00 | 0.00 | 3A7 |
| ATOM | 2472 | CD2 | LEU | 351 | 7.441  | -35.402 | 31.865 | 1.00 | 0.00 | 3A7 |
| ATOM | 2473 | C   | LEU | 351 | 4.203  | -32.710 | 33.432 | 1.00 | 0.00 | 3A7 |
| ATOM | 2474 | O   | LEU | 351 | 3.248  | -32.996 | 32.716 | 1.00 | 0.00 | 3A7 |
| ATOM | 2475 | N   | GLN | 352 | 4.059  | -31.949 | 34.546 | 1.00 | 0.00 | 3A7 |
| ATOM | 2476 | CA  | GLN | 352 | 2.775  | -31.491 | 35.037 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2477 | CB  | GLN | 352 | 2.625  | -31.677 | 36.565 | 1.00 | 0.00 | 3A7 |
| ATOM | 2478 | CG  | GLN | 352 | 2.109  | -33.072 | 36.977 | 1.00 | 0.00 | 3A7 |
| ATOM | 2479 | CD  | GLN | 352 | 3.125  | -34.176 | 36.678 | 1.00 | 0.00 | 3A7 |
| ATOM | 2480 | OE1 | GLN | 352 | 2.971  | -34.938 | 35.716 | 1.00 | 0.00 | 3A7 |
| ATOM | 2481 | NE2 | GLN | 352 | 4.173  | -34.268 | 37.551 | 1.00 | 0.00 | 3A7 |
| ATOM | 2482 | C   | GLN | 352 | 2.540  | -30.043 | 34.711 | 1.00 | 0.00 | 3A7 |
| ATOM | 2483 | O   | GLN | 352 | 1.702  | -29.394 | 35.333 | 1.00 | 0.00 | 3A7 |
| ATOM | 2484 | N   | LEU | 353 | 3.254  | -29.494 | 33.712 | 1.00 | 0.00 | 3A7 |
| ATOM | 2485 | CA  | LEU | 353 | 3.130  | -28.104 | 33.338 | 1.00 | 0.00 | 3A7 |
| ATOM | 2486 | CB  | LEU | 353 | 4.489  | -27.396 | 33.371 | 1.00 | 0.00 | 3A7 |
| ATOM | 2487 | CG  | LEU | 353 | 4.991  | -27.076 | 34.789 | 1.00 | 0.00 | 3A7 |
| ATOM | 2488 | CD1 | LEU | 353 | 6.496  | -26.787 | 34.712 | 1.00 | 0.00 | 3A7 |
| ATOM | 2489 | CD2 | LEU | 353 | 4.215  | -25.911 | 35.433 | 1.00 | 0.00 | 3A7 |
| ATOM | 2490 | C   | LEU | 353 | 2.588  | -28.000 | 31.951 | 1.00 | 0.00 | 3A7 |
| ATOM | 2491 | O   | LEU | 353 | 3.198  | -27.396 | 31.071 | 1.00 | 0.00 | 3A7 |
| ATOM | 2492 | N   | GLU | 354 | 1.380  | -28.556 | 31.747 | 1.00 | 0.00 | 3A7 |
| ATOM | 2493 | CA  | GLU | 354 | 0.702  | -28.679 | 30.481 | 1.00 | 0.00 | 3A7 |
| ATOM | 2494 | CB  | GLU | 354 | -0.697 | -29.284 | 30.692 | 1.00 | 0.00 | 3A7 |
| ATOM | 2495 | CG  | GLU | 354 | -0.745 | -30.790 | 31.013 | 1.00 | 0.00 | 3A7 |
| ATOM | 2496 | CD  | GLU | 354 | -0.273 | -31.081 | 32.431 | 1.00 | 0.00 | 3A7 |
| ATOM | 2497 | OE1 | GLU | 354 | 0.614  | -31.962 | 32.579 | 1.00 | 0.00 | 3A7 |
| ATOM | 2498 | OE2 | GLU | 354 | -0.801 | -30.446 | 33.382 | 1.00 | 0.00 | 3A7 |
| ATOM | 2499 | C   | GLU | 354 | 0.533  | -27.384 | 29.710 | 1.00 | 0.00 | 3A7 |
| ATOM | 2500 | O   | GLU | 354 | 0.869  | -27.315 | 28.531 | 1.00 | 0.00 | 3A7 |
| ATOM | 2501 | N   | TYR | 355 | 0.017  | -26.319 | 30.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 2502 | CA  | TYR | 355 | -0.255 | -25.056 | 29.708 | 1.00 | 0.00 | 3A7 |
| ATOM | 2503 | CB  | TYR | 355 | -1.107 | -24.126 | 30.584 | 1.00 | 0.00 | 3A7 |
| ATOM | 2504 | CG  | TYR | 355 | -2.413 | -24.797 | 30.922 | 1.00 | 0.00 | 3A7 |
| ATOM | 2505 | CD1 | TYR | 355 | -2.853 | -24.843 | 32.245 | 1.00 | 0.00 | 3A7 |
| ATOM | 2506 | CD2 | TYR | 355 | -3.183 | -25.427 | 29.938 | 1.00 | 0.00 | 3A7 |
| ATOM | 2507 | CE1 | TYR | 355 | -4.029 | -25.504 | 32.585 | 1.00 | 0.00 | 3A7 |
| ATOM | 2508 | CE2 | TYR | 355 | -4.354 | -26.101 | 30.275 | 1.00 | 0.00 | 3A7 |
| ATOM | 2509 | CZ  | TYR | 355 | -4.779 | -26.138 | 31.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 2510 | OH  | TYR | 355 | -5.972 | -26.813 | 31.940 | 1.00 | 0.00 | 3A7 |
| ATOM | 2511 | C   | TYR | 355 | 1.014  | -24.314 | 29.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 2512 | O   | TYR | 355 | 1.093  | -23.672 | 28.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 2513 | N   | LEU | 356 | 2.069  | -24.432 | 30.194 | 1.00 | 0.00 | 3A7 |
| ATOM | 2514 | CA  | LEU | 356 | 3.372  | -23.853 | 29.929 | 1.00 | 0.00 | 3A7 |
| ATOM | 2515 | CB  | LEU | 356 | 4.307  | -24.000 | 31.136 | 1.00 | 0.00 | 3A7 |
| ATOM | 2516 | CG  | LEU | 356 | 5.331  | -22.859 | 31.211 | 1.00 | 0.00 | 3A7 |
| ATOM | 2517 | CD1 | LEU | 356 | 5.499  | -22.429 | 32.674 | 1.00 | 0.00 | 3A7 |
| ATOM | 2518 | CD2 | LEU | 356 | 6.699  | -23.187 | 30.588 | 1.00 | 0.00 | 3A7 |
| ATOM | 2519 | C   | LEU | 356 | 4.082  | -24.430 | 28.735 | 1.00 | 0.00 | 3A7 |
| ATOM | 2520 | O   | LEU | 356 | 4.610  | -23.709 | 27.891 | 1.00 | 0.00 | 3A7 |
| ATOM | 2521 | N   | ASP | 357 | 4.076  | -25.778 | 28.619 | 1.00 | 0.00 | 3A7 |
| ATOM | 2522 | CA  | ASP | 357 | 4.652  | -26.516 | 27.513 | 1.00 | 0.00 | 3A7 |
| ATOM | 2523 | CB  | ASP | 357 | 4.362  | -28.050 | 27.598 | 1.00 | 0.00 | 3A7 |
| ATOM | 2524 | CG  | ASP | 357 | 5.259  | -28.771 | 28.597 | 1.00 | 0.00 | 3A7 |
| ATOM | 2525 | OD1 | ASP | 357 | 5.958  | -29.726 | 28.159 | 1.00 | 0.00 | 3A7 |
| ATOM | 2526 | OD2 | ASP | 357 | 5.258  | -28.397 | 29.796 | 1.00 | 0.00 | 3A7 |
| ATOM | 2527 | C   | ASP | 357 | 4.055  | -26.136 | 26.182 | 1.00 | 0.00 | 3A7 |
| ATOM | 2528 | O   | ASP | 357 | 4.748  | -25.985 | 25.183 | 1.00 | 0.00 | 3A7 |
| ATOM | 2529 | N   | MET | 358 | 2.719  | -25.956 | 26.163 | 1.00 | 0.00 | 3A7 |
| ATOM | 2530 | CA  | MET | 358 | 1.969  | -25.573 | 24.997 | 1.00 | 0.00 | 3A7 |
| ATOM | 2531 | CB  | MET | 358 | 0.466  | -25.711 | 25.263 | 1.00 | 0.00 | 3A7 |
| ATOM | 2532 | CG  | MET | 358 | 0.027  | -27.178 | 25.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 2533 | SD  | MET | 358 | -1.535 | -27.420 | 26.341 | 1.00 | 0.00 | 3A7 |
| ATOM | 2534 | CE  | MET | 358 | -2.631 | -26.461 | 25.262 | 1.00 | 0.00 | 3A7 |
| ATOM | 2535 | C   | MET | 358 | 2.269  | -24.149 | 24.601 | 1.00 | 0.00 | 3A7 |
| ATOM | 2536 | O   | MET | 358 | 2.344  | -23.825 | 23.421 | 1.00 | 0.00 | 3A7 |
| ATOM | 2537 | N   | VAL | 359 | 2.505  | -23.255 | 25.594 | 1.00 | 0.00 | 3A7 |
| ATOM | 2538 | CA  | VAL | 359 | 2.885  | -21.869 | 25.376 | 1.00 | 0.00 | 3A7 |
| ATOM | 2539 | CB  | VAL | 359 | 2.885  | -21.083 | 26.684 | 1.00 | 0.00 | 3A7 |
| ATOM | 2540 | CG1 | VAL | 359 | 3.710  | -19.776 | 26.626 | 1.00 | 0.00 | 3A7 |
| ATOM | 2541 | CG2 | VAL | 359 | 1.412  | -20.783 | 27.005 | 1.00 | 0.00 | 3A7 |
| ATOM | 2542 | C   | VAL | 359 | 4.233  | -21.791 | 24.701 | 1.00 | 0.00 | 3A7 |
| ATOM | 2543 | O   | VAL | 359 | 4.408  | -21.063 | 23.725 | 1.00 | 0.00 | 3A7 |
| ATOM | 2544 | N   | VAL | 360 | 5.224  | -22.575 | 25.182 | 1.00 | 0.00 | 3A7 |
| ATOM | 2545 | CA  | VAL | 360 | 6.556  | -22.600 | 24.616 | 1.00 | 0.00 | 3A7 |
| ATOM | 2546 | CB  | VAL | 360 | 7.506  | -23.421 | 25.479 | 1.00 | 0.00 | 3A7 |
| ATOM | 2547 | CG1 | VAL | 360 | 8.897  | -23.573 | 24.831 | 1.00 | 0.00 | 3A7 |
| ATOM | 2548 | CG2 | VAL | 360 | 7.633  | -22.713 | 26.844 | 1.00 | 0.00 | 3A7 |



|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2549 | C   | VAL | 360 | 6.520  | -23.153 | 23.207 | 1.00 | 0.00 | 3A7 |
| ATOM | 2550 | O   | VAL | 360 | 7.168  | -22.609 | 22.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 2551 | N   | ASN | 361 | 5.711  | -24.208 | 22.949 | 1.00 | 0.00 | 3A7 |
| ATOM | 2552 | CA  | ASN | 361 | 5.556  | -24.789 | 21.630 | 1.00 | 0.00 | 3A7 |
| ATOM | 2553 | CB  | ASN | 361 | 4.650  | -26.030 | 21.669 | 1.00 | 0.00 | 3A7 |
| ATOM | 2554 | CG  | ASN | 361 | 5.417  | -27.219 | 22.258 | 1.00 | 0.00 | 3A7 |
| ATOM | 2555 | OD1 | ASN | 361 | 6.641  | -27.329 | 22.121 | 1.00 | 0.00 | 3A7 |
| ATOM | 2556 | ND2 | ASN | 361 | 4.654  | -28.135 | 22.930 | 1.00 | 0.00 | 3A7 |
| ATOM | 2557 | C   | ASN | 361 | 4.952  | -23.808 | 20.655 | 1.00 | 0.00 | 3A7 |
| ATOM | 2558 | O   | ASN | 361 | 5.410  | -23.694 | 19.523 | 1.00 | 0.00 | 3A7 |
| ATOM | 2559 | N   | GLU | 362 | 3.925  | -23.044 | 21.087 | 1.00 | 0.00 | 3A7 |
| ATOM | 2560 | CA  | GLU | 362 | 3.338  | -21.994 | 20.287 | 1.00 | 0.00 | 3A7 |
| ATOM | 2561 | CB  | GLU | 362 | 2.013  | -21.499 | 20.896 | 1.00 | 0.00 | 3A7 |
| ATOM | 2562 | CG  | GLU | 362 | 1.224  | -20.515 | 20.011 | 1.00 | 0.00 | 3A7 |
| ATOM | 2563 | CD  | GLU | 362 | 0.583  | -21.183 | 18.798 | 1.00 | 0.00 | 3A7 |
| ATOM | 2564 | OE1 | GLU | 362 | 0.987  | -22.314 | 18.429 | 1.00 | 0.00 | 3A7 |
| ATOM | 2565 | OE2 | GLU | 362 | -0.309 | -20.534 | 18.190 | 1.00 | 0.00 | 3A7 |
| ATOM | 2566 | C   | GLU | 362 | 4.241  | -20.837 | 20.000 | 1.00 | 0.00 | 3A7 |
| ATOM | 2567 | O   | GLU | 362 | 4.205  | -20.266 | 18.913 | 1.00 | 0.00 | 3A7 |
| ATOM | 2568 | N   | THR | 363 | 5.135  | -20.478 | 20.946 | 1.00 | 0.00 | 3A7 |
| ATOM | 2569 | CA  | THR | 363 | 6.090  | -19.416 | 20.720 | 1.00 | 0.00 | 3A7 |
| ATOM | 2570 | CB  | THR | 363 | 6.793  | -19.002 | 21.991 | 1.00 | 0.00 | 3A7 |
| ATOM | 2571 | OG1 | THR | 363 | 5.804  | -18.623 | 22.938 | 1.00 | 0.00 | 3A7 |
| ATOM | 2572 | CG2 | THR | 363 | 7.691  | -17.778 | 21.706 | 1.00 | 0.00 | 3A7 |
| ATOM | 2573 | C   | THR | 363 | 7.091  | -19.831 | 19.666 | 1.00 | 0.00 | 3A7 |
| ATOM | 2574 | O   | THR | 363 | 7.464  | -19.042 | 18.805 | 1.00 | 0.00 | 3A7 |
| ATOM | 2575 | N   | LEU | 364 | 7.504  | -21.115 | 19.676 | 1.00 | 0.00 | 3A7 |
| ATOM | 2576 | CA  | LEU | 364 | 8.417  | -21.641 | 18.695 | 1.00 | 0.00 | 3A7 |
| ATOM | 2577 | CB  | LEU | 364 | 8.957  | -23.014 | 19.086 | 1.00 | 0.00 | 3A7 |
| ATOM | 2578 | CG  | LEU | 364 | 9.921  | -23.018 | 20.283 | 1.00 | 0.00 | 3A7 |
| ATOM | 2579 | CD1 | LEU | 364 | 10.242 | -24.462 | 20.696 | 1.00 | 0.00 | 3A7 |
| ATOM | 2580 | CD2 | LEU | 364 | 11.219 | -22.259 | 19.974 | 1.00 | 0.00 | 3A7 |
| ATOM | 2581 | C   | LEU | 364 | 7.769  | -21.746 | 17.338 | 1.00 | 0.00 | 3A7 |
| ATOM | 2582 | O   | LEU | 364 | 8.410  | -21.492 | 16.324 | 1.00 | 0.00 | 3A7 |
| ATOM | 2583 | N   | ARG | 365 | 6.467  | -22.094 | 17.264 | 1.00 | 0.00 | 3A7 |
| ATOM | 2584 | CA  | ARG | 365 | 5.743  | -22.109 | 16.003 | 1.00 | 0.00 | 3A7 |
| ATOM | 2585 | CB  | ARG | 365 | 4.300  | -22.612 | 16.169 | 1.00 | 0.00 | 3A7 |
| ATOM | 2586 | CG  | ARG | 365 | 3.614  | -22.980 | 14.858 | 1.00 | 0.00 | 3A7 |
| ATOM | 2587 | CD  | ARG | 365 | 2.117  | -23.285 | 15.005 | 1.00 | 0.00 | 3A7 |
| ATOM | 2588 | NE  | ARG | 365 | 1.371  | -21.987 | 15.068 | 1.00 | 0.00 | 3A7 |
| ATOM | 2589 | CZ  | ARG | 365 | 0.011  | -21.942 | 15.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 2590 | NH1 | ARG | 365 | -0.637 | -20.742 | 15.124 | 1.00 | 0.00 | 3A7 |
| ATOM | 2591 | NH2 | ARG | 365 | -0.703 | -23.084 | 15.418 | 1.00 | 0.00 | 3A7 |
| ATOM | 2592 | C   | ARG | 365 | 5.648  | -20.756 | 15.371 | 1.00 | 0.00 | 3A7 |
| ATOM | 2593 | O   | ARG | 365 | 5.941  | -20.573 | 14.192 | 1.00 | 0.00 | 3A7 |
| ATOM | 2594 | N   | LEU | 366 | 5.239  | -19.760 | 16.176 | 1.00 | 0.00 | 3A7 |
| ATOM | 2595 | CA  | LEU | 366 | 5.030  | -18.410 | 15.729 | 1.00 | 0.00 | 3A7 |
| ATOM | 2596 | CB  | LEU | 366 | 4.204  | -17.608 | 16.752 | 1.00 | 0.00 | 3A7 |
| ATOM | 2597 | CG  | LEU | 366 | 3.017  | -16.833 | 16.122 | 1.00 | 0.00 | 3A7 |
| ATOM | 2598 | CD1 | LEU | 366 | 2.029  | -16.361 | 17.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 2599 | CD2 | LEU | 366 | 3.452  | -15.648 | 15.240 | 1.00 | 0.00 | 3A7 |
| ATOM | 2600 | C   | LEU | 366 | 6.295  | -17.670 | 15.380 | 1.00 | 0.00 | 3A7 |
| ATOM | 2601 | O   | LEU | 366 | 6.339  | -16.992 | 14.359 | 1.00 | 0.00 | 3A7 |
| ATOM | 2602 | N   | PHE | 367 | 7.367  | -17.798 | 16.193 | 1.00 | 0.00 | 3A7 |
| ATOM | 2603 | CA  | PHE | 367 | 8.619  | -17.136 | 15.897 | 1.00 | 0.00 | 3A7 |
| ATOM | 2604 | CB  | PHE | 367 | 8.999  | -16.072 | 16.907 | 1.00 | 0.00 | 3A7 |
| ATOM | 2605 | CG  | PHE | 367 | 7.886  | -15.081 | 17.042 | 1.00 | 0.00 | 3A7 |
| ATOM | 2606 | CD1 | PHE | 367 | 6.921  | -15.250 | 18.035 | 1.00 | 0.00 | 3A7 |
| ATOM | 2607 | CD2 | PHE | 367 | 7.781  | -13.998 | 16.170 | 1.00 | 0.00 | 3A7 |
| ATOM | 2608 | CE1 | PHE | 367 | 5.855  | -14.365 | 18.137 | 1.00 | 0.00 | 3A7 |
| ATOM | 2609 | CE2 | PHE | 367 | 6.723  | -13.100 | 16.285 | 1.00 | 0.00 | 3A7 |
| ATOM | 2610 | CZ  | PHE | 367 | 5.757  | -13.284 | 17.269 | 1.00 | 0.00 | 3A7 |
| ATOM | 2611 | C   | PHE | 367 | 9.740  | -18.121 | 15.878 | 1.00 | 0.00 | 3A7 |
| ATOM | 2612 | O   | PHE | 367 | 10.525 | -18.207 | 16.823 | 1.00 | 0.00 | 3A7 |
| ATOM | 2613 | N   | PRO | 368 | 9.897  | -18.877 | 14.814 | 1.00 | 0.00 | 3A7 |
| ATOM | 2614 | CA  | PRO | 368 | 10.926 | -19.868 | 14.730 | 1.00 | 0.00 | 3A7 |
| ATOM | 2615 | CD  | PRO | 368 | 8.891  | -19.039 | 13.788 | 1.00 | 0.00 | 3A7 |
| ATOM | 2616 | CB  | PRO | 368 | 10.570 | -20.710 | 13.544 | 1.00 | 0.00 | 3A7 |
| ATOM | 2617 | CG  | PRO | 368 | 9.531  | -19.942 | 12.757 | 1.00 | 0.00 | 3A7 |
| ATOM | 2618 | C   | PRO | 368 | 12.257 | -19.200 | 14.589 | 1.00 | 0.00 | 3A7 |
| ATOM | 2619 | O   | PRO | 368 | 12.479 | -18.434 | 13.657 | 1.00 | 0.00 | 3A7 |
| ATOM | 2620 | N   | VAL | 369 | 13.143 | -19.481 | 15.561 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2621 | CA  | VAL | 369 | 14.427 | -18.858 | 15.709 | 1.00 | 0.00 | 3A7 |
| ATOM | 2622 | CB  | VAL | 369 | 15.058 | -19.329 | 16.991 | 1.00 | 0.00 | 3A7 |
| ATOM | 2623 | CG1 | VAL | 369 | 16.449 | -18.705 | 17.115 | 1.00 | 0.00 | 3A7 |
| ATOM | 2624 | CG2 | VAL | 369 | 14.135 | -18.876 | 18.133 | 1.00 | 0.00 | 3A7 |
| ATOM | 2625 | C   | VAL | 369 | 15.330 | -19.141 | 14.529 | 1.00 | 0.00 | 3A7 |
| ATOM | 2626 | O   | VAL | 369 | 16.105 | -18.284 | 14.109 | 1.00 | 0.00 | 3A7 |
| ATOM | 2627 | N   | ALA | 370 | 15.232 | -20.349 | 13.946 | 1.00 | 0.00 | 3A7 |
| ATOM | 2628 | CA  | ALA | 370 | 15.984 | -20.686 | 12.775 | 1.00 | 0.00 | 3A7 |
| ATOM | 2629 | CB  | ALA | 370 | 16.677 | -22.035 | 12.966 | 1.00 | 0.00 | 3A7 |
| ATOM | 2630 | C   | ALA | 370 | 15.038 | -20.739 | 11.619 | 1.00 | 0.00 | 3A7 |
| ATOM | 2631 | O   | ALA | 370 | 14.503 | -21.792 | 11.309 | 1.00 | 0.00 | 3A7 |
| ATOM | 2632 | N   | MET | 371 | 14.813 | -19.597 | 10.938 | 1.00 | 0.00 | 3A7 |
| ATOM | 2633 | CA  | MET | 371 | 13.787 | -19.436 | 9.924  | 1.00 | 0.00 | 3A7 |
| ATOM | 2634 | CB  | MET | 371 | 13.599 | -17.940 | 9.616  | 1.00 | 0.00 | 3A7 |
| ATOM | 2635 | CG  | MET | 371 | 14.852 | -17.053 | 9.800  | 1.00 | 0.00 | 3A7 |
| ATOM | 2636 | SD  | MET | 371 | 16.175 | -17.276 | 8.566  | 1.00 | 0.00 | 3A7 |
| ATOM | 2637 | CE  | MET | 371 | 15.303 | -16.484 | 7.182  | 1.00 | 0.00 | 3A7 |
| ATOM | 2638 | C   | MET | 371 | 14.093 | -20.142 | 8.625  | 1.00 | 0.00 | 3A7 |
| ATOM | 2639 | O   | MET | 371 | 13.208 | -20.260 | 7.783  | 1.00 | 0.00 | 3A7 |
| ATOM | 2640 | N   | ARG | 372 | 15.346 | -20.621 | 8.432  | 1.00 | 0.00 | 3A7 |
| ATOM | 2641 | CA  | ARG | 372 | 15.716 | -21.368 | 7.254  | 1.00 | 0.00 | 3A7 |
| ATOM | 2642 | CB  | ARG | 372 | 16.208 | -20.480 | 6.088  | 1.00 | 0.00 | 3A7 |
| ATOM | 2643 | CG  | ARG | 372 | 15.140 | -19.769 | 5.248  | 1.00 | 0.00 | 3A7 |
| ATOM | 2644 | CD  | ARG | 372 | 15.828 | -19.020 | 4.096  | 1.00 | 0.00 | 3A7 |
| ATOM | 2645 | NE  | ARG | 372 | 14.871 | -18.673 | 2.996  | 1.00 | 0.00 | 3A7 |
| ATOM | 2646 | CZ  | ARG | 372 | 14.486 | -19.599 | 2.066  | 1.00 | 0.00 | 3A7 |
| ATOM | 2647 | NH1 | ARG | 372 | 13.971 | -19.194 | 0.870  | 1.00 | 0.00 | 3A7 |
| ATOM | 2648 | NH2 | ARG | 372 | 14.646 | -20.930 | 2.301  | 1.00 | 0.00 | 3A7 |
| ATOM | 2649 | C   | ARG | 372 | 16.832 | -22.309 | 7.639  | 1.00 | 0.00 | 3A7 |
| ATOM | 2650 | O   | ARG | 372 | 17.619 | -22.029 | 8.542  | 1.00 | 0.00 | 3A7 |
| ATOM | 2651 | N   | LEU | 373 | 16.916 | -23.453 | 6.907  | 1.00 | 0.00 | 3A7 |
| ATOM | 2652 | CA  | LEU | 373 | 17.947 | -24.462 | 7.034  | 1.00 | 0.00 | 3A7 |
| ATOM | 2653 | CB  | LEU | 373 | 17.400 | -25.879 | 7.360  | 1.00 | 0.00 | 3A7 |
| ATOM | 2654 | CG  | LEU | 373 | 16.633 | -26.016 | 8.700  | 1.00 | 0.00 | 3A7 |
| ATOM | 2655 | CD1 | LEU | 373 | 17.347 | -25.305 | 9.860  | 1.00 | 0.00 | 3A7 |
| ATOM | 2656 | CD2 | LEU | 373 | 15.150 | -25.605 | 8.611  | 1.00 | 0.00 | 3A7 |
| ATOM | 2657 | C   | LEU | 373 | 18.641 | -24.532 | 5.697  | 1.00 | 0.00 | 3A7 |
| ATOM | 2658 | O   | LEU | 373 | 18.145 | -23.979 | 4.717  | 1.00 | 0.00 | 3A7 |
| ATOM | 2659 | N   | GLU | 374 | 19.806 | -25.232 | 5.619  | 1.00 | 0.00 | 3A7 |
| ATOM | 2660 | CA  | GLU | 374 | 20.496 | -25.477 | 4.356  | 1.00 | 0.00 | 3A7 |
| ATOM | 2661 | CB  | GLU | 374 | 21.788 | -24.637 | 4.153  | 1.00 | 0.00 | 3A7 |
| ATOM | 2662 | CG  | GLU | 374 | 21.575 | -23.121 | 4.279  | 1.00 | 0.00 | 3A7 |
| ATOM | 2663 | CD  | GLU | 374 | 22.909 | -22.422 | 4.038  | 1.00 | 0.00 | 3A7 |
| ATOM | 2664 | OE1 | GLU | 374 | 23.435 | -21.801 | 5.000  | 1.00 | 0.00 | 3A7 |
| ATOM | 2665 | OE2 | GLU | 374 | 23.420 | -22.501 | 2.889  | 1.00 | 0.00 | 3A7 |
| ATOM | 2666 | C   | GLU | 374 | 20.862 | -26.936 | 4.222  | 1.00 | 0.00 | 3A7 |
| ATOM | 2667 | O   | GLU | 374 | 21.393 | -27.553 | 5.141  | 1.00 | 0.00 | 3A7 |
| ATOM | 2668 | N   | ARG | 375 | 20.591 | -27.510 | 3.026  | 1.00 | 0.00 | 3A7 |
| ATOM | 2669 | CA  | ARG | 375 | 20.879 | -28.878 | 2.666  | 1.00 | 0.00 | 3A7 |
| ATOM | 2670 | CB  | ARG | 375 | 19.614 | -29.770 | 2.636  | 1.00 | 0.00 | 3A7 |
| ATOM | 2671 | CG  | ARG | 375 | 19.033 | -30.018 | 4.037  | 1.00 | 0.00 | 3A7 |
| ATOM | 2672 | CD  | ARG | 375 | 17.789 | -30.919 | 4.035  | 1.00 | 0.00 | 3A7 |
| ATOM | 2673 | NE  | ARG | 375 | 17.499 | -31.381 | 5.436  | 1.00 | 0.00 | 3A7 |
| ATOM | 2674 | CZ  | ARG | 375 | 16.930 | -30.590 | 6.396  | 1.00 | 0.00 | 3A7 |
| ATOM | 2675 | NH1 | ARG | 375 | 16.734 | -31.096 | 7.650  | 1.00 | 0.00 | 3A7 |
| ATOM | 2676 | NH2 | ARG | 375 | 16.558 | -29.307 | 6.125  | 1.00 | 0.00 | 3A7 |
| ATOM | 2677 | C   | ARG | 375 | 21.494 | -28.826 | 1.293  | 1.00 | 0.00 | 3A7 |
| ATOM | 2678 | O   | ARG | 375 | 21.347 | -27.846 | 0.569  | 1.00 | 0.00 | 3A7 |
| ATOM | 2679 | N   | VAL | 376 | 22.225 | -29.890 | 0.889  | 1.00 | 0.00 | 3A7 |
| ATOM | 2680 | CA  | VAL | 376 | 22.836 | -29.949 | -0.420 | 1.00 | 0.00 | 3A7 |
| ATOM | 2681 | CB  | VAL | 376 | 24.347 | -29.725 | -0.397 | 1.00 | 0.00 | 3A7 |
| ATOM | 2682 | CG1 | VAL | 376 | 24.936 | -29.796 | -1.822 | 1.00 | 0.00 | 3A7 |
| ATOM | 2683 | CG2 | VAL | 376 | 24.638 | -28.346 | 0.234  | 1.00 | 0.00 | 3A7 |
| ATOM | 2684 | C   | VAL | 376 | 22.508 | -31.316 | -0.934 | 1.00 | 0.00 | 3A7 |
| ATOM | 2685 | O   | VAL | 376 | 22.653 | -32.316 | -0.233 | 1.00 | 0.00 | 3A7 |
| ATOM | 2686 | N   | CYS | 377 | 22.071 | -31.397 | -2.212 | 1.00 | 0.00 | 3A7 |
| ATOM | 2687 | CA  | CYS | 377 | 21.721 | -32.642 | -2.851 | 1.00 | 0.00 | 3A7 |
| ATOM | 2688 | CB  | CYS | 377 | 20.821 | -32.435 | -4.083 | 1.00 | 0.00 | 3A7 |
| ATOM | 2689 | SG  | CYS | 377 | 19.174 | -31.876 | -3.569 | 1.00 | 0.00 | 3A7 |
| ATOM | 2690 | C   | CYS | 377 | 22.964 | -33.392 | -3.254 | 1.00 | 0.00 | 3A7 |
| ATOM | 2691 | O   | CYS | 377 | 23.919 | -32.843 | -3.794 | 1.00 | 0.00 | 3A7 |
| ATOM | 2692 | N   | LYS | 378 | 22.964 | -34.705 | -2.955 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |         |      |      |     |
|------|------|-----|-----|-----|--------|---------|---------|------|------|-----|
| ATOM | 2693 | CA  | LYS | 378 | 24.083 | -35.594 | -3.143  | 1.00 | 0.00 | 3A7 |
| ATOM | 2694 | CB  | LYS | 378 | 24.073 | -36.718 | -2.075  | 1.00 | 0.00 | 3A7 |
| ATOM | 2695 | CG  | LYS | 378 | 23.127 | -36.428 | -0.894  | 1.00 | 0.00 | 3A7 |
| ATOM | 2696 | CD  | LYS | 378 | 23.024 | -37.592 | 0.101   | 1.00 | 0.00 | 3A7 |
| ATOM | 2697 | CE  | LYS | 378 | 21.948 | -37.375 | 1.174   | 1.00 | 0.00 | 3A7 |
| ATOM | 2698 | NZ  | LYS | 378 | 22.223 | -36.159 | 1.974   | 1.00 | 0.00 | 3A7 |
| ATOM | 2699 | C   | LYS | 378 | 24.040 | -36.202 | -4.524  | 1.00 | 0.00 | 3A7 |
| ATOM | 2700 | O   | LYS | 378 | 25.062 | -36.609 | -5.075  | 1.00 | 0.00 | 3A7 |
| ATOM | 2701 | N   | LYS | 379 | 22.814 | -36.285 | -5.081  | 1.00 | 0.00 | 3A7 |
| ATOM | 2702 | CA  | LYS | 379 | 22.547 | -36.939 | -6.329  | 1.00 | 0.00 | 3A7 |
| ATOM | 2703 | CB  | LYS | 379 | 22.121 | -38.417 | -6.127  | 1.00 | 0.00 | 3A7 |
| ATOM | 2704 | CG  | LYS | 379 | 20.935 | -38.609 | -5.161  | 1.00 | 0.00 | 3A7 |
| ATOM | 2705 | CD  | LYS | 379 | 20.582 | -40.083 | -4.899  | 1.00 | 0.00 | 3A7 |
| ATOM | 2706 | CE  | LYS | 379 | 21.665 | -40.842 | -4.120  | 1.00 | 0.00 | 3A7 |
| ATOM | 2707 | NZ  | LYS | 379 | 21.236 | -42.233 | -3.850  | 1.00 | 0.00 | 3A7 |
| ATOM | 2708 | C   | LYS | 379 | 21.450 | -36.155 | -6.981  | 1.00 | 0.00 | 3A7 |
| ATOM | 2709 | O   | LYS | 379 | 21.014 | -35.119 | -6.483  | 1.00 | 0.00 | 3A7 |
| ATOM | 2710 | N   | ASP | 380 | 20.951 | -36.650 | -8.134  | 1.00 | 0.00 | 3A7 |
| ATOM | 2711 | CA  | ASP | 380 | 19.820 | -36.071 | -8.818  | 1.00 | 0.00 | 3A7 |
| ATOM | 2712 | CB  | ASP | 380 | 19.811 | -36.404 | -10.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 2713 | CG  | ASP | 380 | 21.092 | -35.921 | -10.999 | 1.00 | 0.00 | 3A7 |
| ATOM | 2714 | OD1 | ASP | 380 | 21.347 | -34.689 | -10.981 | 1.00 | 0.00 | 3A7 |
| ATOM | 2715 | OD2 | ASP | 380 | 21.824 | -36.782 | -11.556 | 1.00 | 0.00 | 3A7 |
| ATOM | 2716 | C   | ASP | 380 | 18.562 | -36.616 | -8.182  | 1.00 | 0.00 | 3A7 |
| ATOM | 2717 | O   | ASP | 380 | 18.496 | -37.798 | -7.848  | 1.00 | 0.00 | 3A7 |
| ATOM | 2718 | N   | VAL | 381 | 17.554 | -35.744 | -7.966  | 1.00 | 0.00 | 3A7 |
| ATOM | 2719 | CA  | VAL | 381 | 16.378 | -36.118 | -7.224  | 1.00 | 0.00 | 3A7 |
| ATOM | 2720 | CB  | VAL | 381 | 16.557 | -35.910 | -5.720  | 1.00 | 0.00 | 3A7 |
| ATOM | 2721 | CG1 | VAL | 381 | 16.853 | -34.439 | -5.360  | 1.00 | 0.00 | 3A7 |
| ATOM | 2722 | CG2 | VAL | 381 | 15.353 | -36.489 | -4.947  | 1.00 | 0.00 | 3A7 |
| ATOM | 2723 | C   | VAL | 381 | 15.248 | -35.308 | -7.781  | 1.00 | 0.00 | 3A7 |
| ATOM | 2724 | O   | VAL | 381 | 15.417 | -34.151 | -8.142  | 1.00 | 0.00 | 3A7 |
| ATOM | 2725 | N   | GLU | 382 | 14.045 | -35.908 | -7.874  | 1.00 | 0.00 | 3A7 |
| ATOM | 2726 | CA  | GLU | 382 | 12.888 | -35.247 | -8.420  | 1.00 | 0.00 | 3A7 |
| ATOM | 2727 | CB  | GLU | 382 | 12.165 | -36.100 | -9.485  | 1.00 | 0.00 | 3A7 |
| ATOM | 2728 | CG  | GLU | 382 | 12.963 | -36.325 | -10.781 | 1.00 | 0.00 | 3A7 |
| ATOM | 2729 | CD  | GLU | 382 | 14.109 | -37.311 | -10.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 2730 | OE1 | GLU | 382 | 13.827 | -38.470 | -10.163 | 1.00 | 0.00 | 3A7 |
| ATOM | 2731 | OE2 | GLU | 382 | 15.281 | -36.921 | -10.822 | 1.00 | 0.00 | 3A7 |
| ATOM | 2732 | C   | GLU | 382 | 11.952 | -34.980 | -7.271  | 1.00 | 0.00 | 3A7 |
| ATOM | 2733 | O   | GLU | 382 | 11.531 | -35.909 | -6.587  | 1.00 | 0.00 | 3A7 |
| ATOM | 2734 | N   | ILE | 383 | 11.615 | -33.690 | -7.028  | 1.00 | 0.00 | 3A7 |
| ATOM | 2735 | CA  | ILE | 383 | 10.762 | -33.270 | -5.937  | 1.00 | 0.00 | 3A7 |
| ATOM | 2736 | CB  | ILE | 383 | 11.449 | -32.299 | -4.973  | 1.00 | 0.00 | 3A7 |
| ATOM | 2737 | CG2 | ILE | 383 | 10.543 | -32.043 | -3.747  | 1.00 | 0.00 | 3A7 |
| ATOM | 2738 | CG1 | ILE | 383 | 12.865 | -32.774 | -4.555  | 1.00 | 0.00 | 3A7 |
| ATOM | 2739 | CD  | ILE | 383 | 12.883 | -34.026 | -3.677  | 1.00 | 0.00 | 3A7 |
| ATOM | 2740 | C   | ILE | 383 | 9.578  | -32.594 | -6.567  | 1.00 | 0.00 | 3A7 |
| ATOM | 2741 | O   | ILE | 383 | 9.686  | -31.493 | -7.103  | 1.00 | 0.00 | 3A7 |
| ATOM | 2742 | N   | ASN | 384 | 8.399  | -33.254 | -6.521  | 1.00 | 0.00 | 3A7 |
| ATOM | 2743 | CA  | ASN | 384 | 7.130  | -32.719 | -6.976  | 1.00 | 0.00 | 3A7 |
| ATOM | 2744 | CB  | ASN | 384 | 6.732  | -31.411 | -6.222  | 1.00 | 0.00 | 3A7 |
| ATOM | 2745 | CG  | ASN | 384 | 5.218  | -31.147 | -6.283  | 1.00 | 0.00 | 3A7 |
| ATOM | 2746 | OD1 | ASN | 384 | 4.758  | -30.251 | -7.000  | 1.00 | 0.00 | 3A7 |
| ATOM | 2747 | ND2 | ASN | 384 | 4.443  | -31.956 | -5.498  | 1.00 | 0.00 | 3A7 |
| ATOM | 2748 | C   | ASN | 384 | 7.100  | -32.504 | -8.480  | 1.00 | 0.00 | 3A7 |
| ATOM | 2749 | O   | ASN | 384 | 6.410  | -31.623 | -8.988  | 1.00 | 0.00 | 3A7 |
| ATOM | 2750 | N   | GLY | 385 | 7.870  | -33.322 | -9.231  | 1.00 | 0.00 | 3A7 |
| ATOM | 2751 | CA  | GLY | 385 | 7.911  | -33.246 | -10.666 | 1.00 | 0.00 | 3A7 |
| ATOM | 2752 | C   | GLY | 385 | 9.013  | -32.342 | -11.156 | 1.00 | 0.00 | 3A7 |
| ATOM | 2753 | O   | GLY | 385 | 9.217  | -32.266 | -12.366 | 1.00 | 0.00 | 3A7 |
| ATOM | 2754 | N   | MET | 386 | 9.762  | -31.631 | -10.264 | 1.00 | 0.00 | 3A7 |
| ATOM | 2755 | CA  | MET | 386 | 10.855 | -30.773 | -10.695 | 1.00 | 0.00 | 3A7 |
| ATOM | 2756 | CB  | MET | 386 | 10.660 | -29.264 | -10.426 | 1.00 | 0.00 | 3A7 |
| ATOM | 2757 | CG  | MET | 386 | 10.337 | -28.845 | -8.990  | 1.00 | 0.00 | 3A7 |
| ATOM | 2758 | SD  | MET | 386 | 9.854  | -27.091 | -8.895  | 1.00 | 0.00 | 3A7 |
| ATOM | 2759 | CE  | MET | 386 | 11.448 | -26.373 | -9.388  | 1.00 | 0.00 | 3A7 |
| ATOM | 2760 | C   | MET | 386 | 12.159 | -31.305 | -10.187 | 1.00 | 0.00 | 3A7 |
| ATOM | 2761 | O   | MET | 386 | 12.335 | -31.654 | -9.025  | 1.00 | 0.00 | 3A7 |
| ATOM | 2762 | N   | PHE | 387 | 13.122 | -31.396 | -11.125 | 1.00 | 0.00 | 3A7 |
| ATOM | 2763 | CA  | PHE | 387 | 14.382 | -32.074 | -10.982 | 1.00 | 0.00 | 3A7 |
| ATOM | 2764 | CB  | PHE | 387 | 14.935 | -32.474 | -12.378 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |         |      |      |     |
|------|------|-----|-----|-----|--------|---------|---------|------|------|-----|
| ATOM | 2765 | CG  | PHE | 387 | 14.102 | -33.505 | -13.091 | 1.00 | 0.00 | 3A7 |
| ATOM | 2766 | CD1 | PHE | 387 | 14.645 | -34.767 | -13.344 | 1.00 | 0.00 | 3A7 |
| ATOM | 2767 | CD2 | PHE | 387 | 12.827 | -33.213 | -13.585 | 1.00 | 0.00 | 3A7 |
| ATOM | 2768 | CE1 | PHE | 387 | 13.920 | -35.727 | -14.045 | 1.00 | 0.00 | 3A7 |
| ATOM | 2769 | CE2 | PHE | 387 | 12.097 | -34.173 | -14.280 | 1.00 | 0.00 | 3A7 |
| ATOM | 2770 | CZ  | PHE | 387 | 12.642 | -35.433 | -14.507 | 1.00 | 0.00 | 3A7 |
| ATOM | 2771 | C   | PHE | 387 | 15.405 | -31.180 | -10.312 | 1.00 | 0.00 | 3A7 |
| ATOM | 2772 | O   | PHE | 387 | 15.631 | -30.043 | -10.726 | 1.00 | 0.00 | 3A7 |
| ATOM | 2773 | N   | ILE | 388 | 16.066 | -31.706 | -9.251  | 1.00 | 0.00 | 3A7 |
| ATOM | 2774 | CA  | ILE | 388 | 17.145 | -31.049 | -8.544  | 1.00 | 0.00 | 3A7 |
| ATOM | 2775 | CB  | ILE | 388 | 16.994 | -31.071 | -7.032  | 1.00 | 0.00 | 3A7 |
| ATOM | 2776 | CG2 | ILE | 388 | 18.144 | -30.276 | -6.387  | 1.00 | 0.00 | 3A7 |
| ATOM | 2777 | CG1 | ILE | 388 | 15.641 | -30.487 | -6.591  | 1.00 | 0.00 | 3A7 |
| ATOM | 2778 | CD  | ILE | 388 | 15.434 | -29.010 | -6.913  | 1.00 | 0.00 | 3A7 |
| ATOM | 2779 | C   | ILE | 388 | 18.438 | -31.746 | -8.935  | 1.00 | 0.00 | 3A7 |
| ATOM | 2780 | O   | ILE | 388 | 18.576 | -32.952 | -8.728  | 1.00 | 0.00 | 3A7 |
| ATOM | 2781 | N   | PRO | 389 | 19.415 | -31.021 | -9.496  | 1.00 | 0.00 | 3A7 |
| ATOM | 2782 | CA  | PRO | 389 | 20.698 | -31.581 | -9.867  | 1.00 | 0.00 | 3A7 |
| ATOM | 2783 | CD  | PRO | 389 | 19.063 | -29.901 | -10.375 | 1.00 | 0.00 | 3A7 |
| ATOM | 2784 | CB  | PRO | 389 | 21.290 | -30.549 | -10.822 | 1.00 | 0.00 | 3A7 |
| ATOM | 2785 | CG  | PRO | 389 | 20.081 | -29.931 | -11.509 | 1.00 | 0.00 | 3A7 |
| ATOM | 2786 | C   | PRO | 389 | 21.614 | -31.785 | -8.684  | 1.00 | 0.00 | 3A7 |
| ATOM | 2787 | O   | PRO | 389 | 21.474 | -31.121 | -7.659  | 1.00 | 0.00 | 3A7 |
| ATOM | 2788 | N   | LYS | 390 | 22.627 | -32.663 | -8.836  | 1.00 | 0.00 | 3A7 |
| ATOM | 2789 | CA  | LYS | 390 | 23.654 | -32.884 | -7.847  | 1.00 | 0.00 | 3A7 |
| ATOM | 2790 | CB  | LYS | 390 | 24.733 | -33.851 | -8.363  | 1.00 | 0.00 | 3A7 |
| ATOM | 2791 | CG  | LYS | 390 | 24.234 | -35.053 | -9.176  | 1.00 | 0.00 | 3A7 |
| ATOM | 2792 | CD  | LYS | 390 | 25.372 | -36.029 | -9.517  | 1.00 | 0.00 | 3A7 |
| ATOM | 2793 | CE  | LYS | 390 | 24.921 | -37.258 | -10.316 | 1.00 | 0.00 | 3A7 |
| ATOM | 2794 | NZ  | LYS | 390 | 23.959 | -38.073 | -9.538  | 1.00 | 0.00 | 3A7 |
| ATOM | 2795 | C   | LYS | 390 | 24.346 | -31.584 | -7.486  | 1.00 | 0.00 | 3A7 |
| ATOM | 2796 | O   | LYS | 390 | 24.631 | -30.776 | -8.366  | 1.00 | 0.00 | 3A7 |
| ATOM | 2797 | N   | GLY | 391 | 24.558 | -31.329 | -6.177  | 1.00 | 0.00 | 3A7 |
| ATOM | 2798 | CA  | GLY | 391 | 25.250 | -30.153 | -5.707  | 1.00 | 0.00 | 3A7 |
| ATOM | 2799 | C   | GLY | 391 | 24.397 | -28.926 | -5.567  | 1.00 | 0.00 | 3A7 |
| ATOM | 2800 | O   | GLY | 391 | 24.924 | -27.848 | -5.320  | 1.00 | 0.00 | 3A7 |
| ATOM | 2801 | N   | VAL | 392 | 23.052 | -29.029 | -5.690  | 1.00 | 0.00 | 3A7 |
| ATOM | 2802 | CA  | VAL | 392 | 22.159 | -27.896 | -5.522  | 1.00 | 0.00 | 3A7 |
| ATOM | 2803 | CB  | VAL | 392 | 20.829 | -28.126 | -6.224  | 1.00 | 0.00 | 3A7 |
| ATOM | 2804 | CG1 | VAL | 392 | 19.765 | -27.062 | -5.883  | 1.00 | 0.00 | 3A7 |
| ATOM | 2805 | CG2 | VAL | 392 | 21.074 | -28.134 | -7.744  | 1.00 | 0.00 | 3A7 |
| ATOM | 2806 | C   | VAL | 392 | 21.922 | -27.684 | -4.050  | 1.00 | 0.00 | 3A7 |
| ATOM | 2807 | O   | VAL | 392 | 21.849 | -28.644 | -3.290  | 1.00 | 0.00 | 3A7 |
| ATOM | 2808 | N   | VAL | 393 | 21.787 | -26.403 | -3.629  | 1.00 | 0.00 | 3A7 |
| ATOM | 2809 | CA  | VAL | 393 | 21.491 | -26.024 | -2.268  | 1.00 | 0.00 | 3A7 |
| ATOM | 2810 | CB  | VAL | 393 | 22.118 | -24.695 | -1.900  | 1.00 | 0.00 | 3A7 |
| ATOM | 2811 | CG1 | VAL | 393 | 21.828 | -24.336 | -0.425  | 1.00 | 0.00 | 3A7 |
| ATOM | 2812 | CG2 | VAL | 393 | 23.636 | -24.785 | -2.160  | 1.00 | 0.00 | 3A7 |
| ATOM | 2813 | C   | VAL | 393 | 19.992 | -25.964 | -2.130  | 1.00 | 0.00 | 3A7 |
| ATOM | 2814 | O   | VAL | 393 | 19.308 | -25.288 | -2.891  | 1.00 | 0.00 | 3A7 |
| ATOM | 2815 | N   | VAL | 394 | 19.457 | -26.712 | -1.145  | 1.00 | 0.00 | 3A7 |
| ATOM | 2816 | CA  | VAL | 394 | 18.049 | -26.825 | -0.864  | 1.00 | 0.00 | 3A7 |
| ATOM | 2817 | CB  | VAL | 394 | 17.609 | -28.282 | -0.810  | 1.00 | 0.00 | 3A7 |
| ATOM | 2818 | CG1 | VAL | 394 | 16.104 | -28.411 | -0.510  | 1.00 | 0.00 | 3A7 |
| ATOM | 2819 | CG2 | VAL | 394 | 17.948 | -28.936 | -2.163  | 1.00 | 0.00 | 3A7 |
| ATOM | 2820 | C   | VAL | 394 | 17.840 | -26.177 | 0.471   | 1.00 | 0.00 | 3A7 |
| ATOM | 2821 | O   | VAL | 394 | 18.601 | -26.423 | 1.400   | 1.00 | 0.00 | 3A7 |
| ATOM | 2822 | N   | MET | 395 | 16.800 | -25.325 | 0.609   | 1.00 | 0.00 | 3A7 |
| ATOM | 2823 | CA  | MET | 395 | 16.529 | -24.656 | 1.856   | 1.00 | 0.00 | 3A7 |
| ATOM | 2824 | CB  | MET | 395 | 16.818 | -23.145 | 1.809   | 1.00 | 0.00 | 3A7 |
| ATOM | 2825 | CG  | MET | 395 | 18.304 | -22.812 | 1.578   | 1.00 | 0.00 | 3A7 |
| ATOM | 2826 | SD  | MET | 395 | 18.747 | -21.101 | 2.015   | 1.00 | 0.00 | 3A7 |
| ATOM | 2827 | CE  | MET | 395 | 17.770 | -20.277 | 0.725   | 1.00 | 0.00 | 3A7 |
| ATOM | 2828 | C   | MET | 395 | 15.093 | -24.885 | 2.216   | 1.00 | 0.00 | 3A7 |
| ATOM | 2829 | O   | MET | 395 | 14.195 | -24.925 | 1.389   | 1.00 | 0.00 | 3A7 |
| ATOM | 2830 | N   | ILE | 396 | 14.842 | -25.076 | 3.515   | 1.00 | 0.00 | 3A7 |
| ATOM | 2831 | CA  | ILE | 396 | 13.536 | -25.356 | 4.059   | 1.00 | 0.00 | 3A7 |
| ATOM | 2832 | CB  | ILE | 396 | 13.599 | -26.610 | 4.904   | 1.00 | 0.00 | 3A7 |
| ATOM | 2833 | CG2 | ILE | 396 | 12.490 | -26.667 | 5.983   | 1.00 | 0.00 | 3A7 |
| ATOM | 2834 | CG1 | ILE | 396 | 13.729 | -27.897 | 4.057   | 1.00 | 0.00 | 3A7 |
| ATOM | 2835 | CD  | ILE | 396 | 15.087 | -28.104 | 3.373   | 1.00 | 0.00 | 3A7 |
| ATOM | 2836 | C   | ILE | 396 | 13.188 | -24.182 | 4.902   | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2837 | O   | ILE | 396 | 13.874 | -23.964 | 5.894  | 1.00 | 0.00 | 3A7 |
| ATOM | 2838 | N   | PRO | 397 | 12.167 | -23.398 | 4.590  | 1.00 | 0.00 | 3A7 |
| ATOM | 2839 | CA  | PRO | 397 | 11.790 | -22.297 | 5.462  | 1.00 | 0.00 | 3A7 |
| ATOM | 2840 | CD  | PRO | 397 | 11.961 | -23.022 | 3.209  | 1.00 | 0.00 | 3A7 |
| ATOM | 2841 | CB  | PRO | 397 | 11.201 | -21.252 | 4.533  | 1.00 | 0.00 | 3A7 |
| ATOM | 2842 | CG  | PRO | 397 | 10.809 | -22.043 | 3.293  | 1.00 | 0.00 | 3A7 |
| ATOM | 2843 | C   | PRO | 397 | 10.834 | -22.717 | 6.544  | 1.00 | 0.00 | 3A7 |
| ATOM | 2844 | O   | PRO | 397 | 9.629  | -22.732 | 6.310  | 1.00 | 0.00 | 3A7 |
| ATOM | 2845 | N   | SER | 398 | 11.352 | -22.981 | 7.767  | 1.00 | 0.00 | 3A7 |
| ATOM | 2846 | CA  | SER | 398 | 10.575 | -23.392 | 8.914  | 1.00 | 0.00 | 3A7 |
| ATOM | 2847 | CB  | SER | 398 | 11.471 | -23.676 | 10.138 | 1.00 | 0.00 | 3A7 |
| ATOM | 2848 | OG  | SER | 398 | 12.135 | -22.517 | 10.613 | 1.00 | 0.00 | 3A7 |
| ATOM | 2849 | C   | SER | 398 | 9.531  | -22.379 | 9.316  | 1.00 | 0.00 | 3A7 |
| ATOM | 2850 | O   | SER | 398 | 8.422  | -22.745 | 9.668  | 1.00 | 0.00 | 3A7 |
| ATOM | 2851 | N   | TYR | 399 | 9.838  | -21.053 | 9.231  | 1.00 | 0.00 | 3A7 |
| ATOM | 2852 | CA  | TYR | 399 | 8.913  | -19.958 | 9.507  | 1.00 | 0.00 | 3A7 |
| ATOM | 2853 | CB  | TYR | 399 | 9.578  | -18.562 | 9.264  | 1.00 | 0.00 | 3A7 |
| ATOM | 2854 | CG  | TYR | 399 | 9.084  | -17.492 | 10.212 | 1.00 | 0.00 | 3A7 |
| ATOM | 2855 | CD1 | TYR | 399 | 9.933  | -16.936 | 11.172 | 1.00 | 0.00 | 3A7 |
| ATOM | 2856 | CD2 | TYR | 399 | 7.775  | -17.008 | 10.123 | 1.00 | 0.00 | 3A7 |
| ATOM | 2857 | CE1 | TYR | 399 | 9.473  | -15.959 | 12.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 2858 | CE2 | TYR | 399 | 7.308  | -16.041 | 11.007 | 1.00 | 0.00 | 3A7 |
| ATOM | 2859 | CZ  | TYR | 399 | 8.156  | -15.520 | 11.975 | 1.00 | 0.00 | 3A7 |
| ATOM | 2860 | OH  | TYR | 399 | 7.673  | -14.553 | 12.880 | 1.00 | 0.00 | 3A7 |
| ATOM | 2861 | C   | TYR | 399 | 7.688  | -20.038 | 8.647  | 1.00 | 0.00 | 3A7 |
| ATOM | 2862 | O   | TYR | 399 | 6.567  | -19.765 | 9.067  | 1.00 | 0.00 | 3A7 |
| ATOM | 2863 | N   | VAL | 400 | 7.911  | -20.472 | 7.398  | 1.00 | 0.00 | 3A7 |
| ATOM | 2864 | CA  | VAL | 400 | 6.877  | -20.616 | 6.436  | 1.00 | 0.00 | 3A7 |
| ATOM | 2865 | CB  | VAL | 400 | 7.444  | -20.658 | 5.045  | 1.00 | 0.00 | 3A7 |
| ATOM | 2866 | CG1 | VAL | 400 | 6.294  | -20.758 | 4.020  | 1.00 | 0.00 | 3A7 |
| ATOM | 2867 | CG2 | VAL | 400 | 8.183  | -19.308 | 4.899  | 1.00 | 0.00 | 3A7 |
| ATOM | 2868 | C   | VAL | 400 | 6.002  | -21.827 | 6.653  | 1.00 | 0.00 | 3A7 |
| ATOM | 2869 | O   | VAL | 400 | 4.781  | -21.734 | 6.547  | 1.00 | 0.00 | 3A7 |
| ATOM | 2870 | N   | LEU | 401 | 6.602  | -22.992 | 6.970  | 1.00 | 0.00 | 3A7 |
| ATOM | 2871 | CA  | LEU | 401 | 5.875  | -24.224 | 7.175  | 1.00 | 0.00 | 3A7 |
| ATOM | 2872 | CB  | LEU | 401 | 6.790  | -25.449 | 7.318  | 1.00 | 0.00 | 3A7 |
| ATOM | 2873 | CG  | LEU | 401 | 8.101  | -25.453 | 6.535  | 1.00 | 0.00 | 3A7 |
| ATOM | 2874 | CD1 | LEU | 401 | 8.877  | -26.722 | 6.915  | 1.00 | 0.00 | 3A7 |
| ATOM | 2875 | CD2 | LEU | 401 | 7.904  | -25.294 | 5.023  | 1.00 | 0.00 | 3A7 |
| ATOM | 2876 | C   | LEU | 401 | 5.031  | -24.186 | 8.449  | 1.00 | 0.00 | 3A7 |
| ATOM | 2877 | O   | LEU | 401 | 3.918  | -24.705 | 8.504  | 1.00 | 0.00 | 3A7 |
| ATOM | 2878 | N   | HIS | 402 | 5.545  | -23.512 | 9.509  | 1.00 | 0.00 | 3A7 |
| ATOM | 2879 | CA  | HIS | 402 | 4.879  | -23.303 | 10.782 | 1.00 | 0.00 | 3A7 |
| ATOM | 2880 | ND1 | HIS | 402 | 7.090  | -24.809 | 12.042 | 1.00 | 0.00 | 3A7 |
| ATOM | 2881 | CG  | HIS | 402 | 6.758  | -23.553 | 12.480 | 1.00 | 0.00 | 3A7 |
| ATOM | 2882 | CB  | HIS | 402 | 5.843  | -22.628 | 11.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 2883 | NE2 | HIS | 402 | 8.734  | -24.122 | 13.375 | 1.00 | 0.00 | 3A7 |
| ATOM | 2884 | CD2 | HIS | 402 | 7.762  | -23.155 | 13.305 | 1.00 | 0.00 | 3A7 |
| ATOM | 2885 | CE1 | HIS | 402 | 8.289  | -25.085 | 12.595 | 1.00 | 0.00 | 3A7 |
| ATOM | 2886 | C   | HIS | 402 | 3.648  | -22.420 | 10.674 | 1.00 | 0.00 | 3A7 |
| ATOM | 2887 | O   | HIS | 402 | 2.844  | -22.343 | 11.602 | 1.00 | 0.00 | 3A7 |
| ATOM | 2888 | N   | HIS | 403 | 3.485  | -21.730 | 9.522  | 1.00 | 0.00 | 3A7 |
| ATOM | 2889 | CA  | HIS | 403 | 2.382  | -20.839 | 9.280  | 1.00 | 0.00 | 3A7 |
| ATOM | 2890 | ND1 | HIS | 403 | 4.537  | -19.115 | 10.966 | 1.00 | 0.00 | 3A7 |
| ATOM | 2891 | CG  | HIS | 403 | 3.389  | -18.746 | 10.299 | 1.00 | 0.00 | 3A7 |
| ATOM | 2892 | CB  | HIS | 403 | 2.858  | -19.394 | 9.048  | 1.00 | 0.00 | 3A7 |
| ATOM | 2893 | NE2 | HIS | 403 | 3.638  | -17.451 | 12.131 | 1.00 | 0.00 | 3A7 |
| ATOM | 2894 | CD2 | HIS | 403 | 2.852  | -17.730 | 11.028 | 1.00 | 0.00 | 3A7 |
| ATOM | 2895 | CE1 | HIS | 403 | 4.638  | -18.308 | 12.051 | 1.00 | 0.00 | 3A7 |
| ATOM | 2896 | C   | HIS | 403 | 1.564  | -21.280 | 8.096  | 1.00 | 0.00 | 3A7 |
| ATOM | 2897 | O   | HIS | 403 | 0.830  | -20.492 | 7.500  | 1.00 | 0.00 | 3A7 |
| ATOM | 2898 | N   | ASP | 404 | 1.605  | -22.588 | 7.740  | 1.00 | 0.00 | 3A7 |
| ATOM | 2899 | CA  | ASP | 404 | 0.811  | -23.143 | 6.662  | 1.00 | 0.00 | 3A7 |
| ATOM | 2900 | CB  | ASP | 404 | 1.274  | -24.585 | 6.322  | 1.00 | 0.00 | 3A7 |
| ATOM | 2901 | CG  | ASP | 404 | 0.584  | -25.218 | 5.103  | 1.00 | 0.00 | 3A7 |
| ATOM | 2902 | OD1 | ASP | 404 | -0.209 | -24.540 | 4.402  | 1.00 | 0.00 | 3A7 |
| ATOM | 2903 | OD2 | ASP | 404 | 0.879  | -26.417 | 4.850  | 1.00 | 0.00 | 3A7 |
| ATOM | 2904 | C   | ASP | 404 | -0.645 | -23.164 | 7.105  | 1.00 | 0.00 | 3A7 |
| ATOM | 2905 | O   | ASP | 404 | -0.941 | -23.809 | 8.108  | 1.00 | 0.00 | 3A7 |
| ATOM | 2906 | N   | PRO | 405 | -1.568 | -22.474 | 6.421  | 1.00 | 0.00 | 3A7 |
| ATOM | 2907 | CA  | PRO | 405 | -2.958 | -22.344 | 6.827  | 1.00 | 0.00 | 3A7 |
| ATOM | 2908 | CD  | PRO | 405 | -1.277 | -21.674 | 5.237  | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2909 | CB  | PRO | 405 | -3.543 | -21.309 | 5.854  | 1.00 | 0.00 | 3A7 |
| ATOM | 2910 | CG  | PRO | 405 | -2.641 | -21.373 | 4.621  | 1.00 | 0.00 | 3A7 |
| ATOM | 2911 | C   | PRO | 405 | -3.739 | -23.646 | 6.756  | 1.00 | 0.00 | 3A7 |
| ATOM | 2912 | O   | PRO | 405 | -4.766 | -23.734 | 7.420  | 1.00 | 0.00 | 3A7 |
| ATOM | 2913 | N   | LYS | 406 | -3.297 | -24.674 | 5.989  | 1.00 | 0.00 | 3A7 |
| ATOM | 2914 | CA  | LYS | 406 | -3.983 | -25.942 | 5.892  | 1.00 | 0.00 | 3A7 |
| ATOM | 2915 | CB  | LYS | 406 | -3.545 | -26.748 | 4.646  | 1.00 | 0.00 | 3A7 |
| ATOM | 2916 | CG  | LYS | 406 | -3.805 | -26.004 | 3.326  | 1.00 | 0.00 | 3A7 |
| ATOM | 2917 | CD  | LYS | 406 | -3.234 | -26.692 | 2.072  | 1.00 | 0.00 | 3A7 |
| ATOM | 2918 | CE  | LYS | 406 | -3.939 | -27.993 | 1.650  | 1.00 | 0.00 | 3A7 |
| ATOM | 2919 | NZ  | LYS | 406 | -3.601 | -29.127 | 2.541  | 1.00 | 0.00 | 3A7 |
| ATOM | 2920 | C   | LYS | 406 | -3.730 | -26.791 | 7.115  | 1.00 | 0.00 | 3A7 |
| ATOM | 2921 | O   | LYS | 406 | -4.554 | -27.622 | 7.479  | 1.00 | 0.00 | 3A7 |
| ATOM | 2922 | N   | TYR | 407 | -2.572 | -26.584 | 7.783  | 1.00 | 0.00 | 3A7 |
| ATOM | 2923 | CA  | TYR | 407 | -2.174 | -27.340 | 8.948  | 1.00 | 0.00 | 3A7 |
| ATOM | 2924 | CB  | TYR | 407 | -0.677 | -27.703 | 8.898  | 1.00 | 0.00 | 3A7 |
| ATOM | 2925 | CG  | TYR | 407 | -0.579 | -28.906 | 8.000  | 1.00 | 0.00 | 3A7 |
| ATOM | 2926 | CD1 | TYR | 407 | -0.674 | -28.783 | 6.613  | 1.00 | 0.00 | 3A7 |
| ATOM | 2927 | CD2 | TYR | 407 | -0.492 | -30.184 | 8.557  | 1.00 | 0.00 | 3A7 |
| ATOM | 2928 | CE1 | TYR | 407 | -0.693 | -29.912 | 5.799  | 1.00 | 0.00 | 3A7 |
| ATOM | 2929 | CE2 | TYR | 407 | -0.483 | -31.314 | 7.746  | 1.00 | 0.00 | 3A7 |
| ATOM | 2930 | CZ  | TYR | 407 | -0.585 | -31.179 | 6.365  | 1.00 | 0.00 | 3A7 |
| ATOM | 2931 | OH  | TYR | 407 | -0.583 | -32.324 | 5.538  | 1.00 | 0.00 | 3A7 |
| ATOM | 2932 | C   | TYR | 407 | -2.474 | -26.584 | 10.218 | 1.00 | 0.00 | 3A7 |
| ATOM | 2933 | O   | TYR | 407 | -2.827 | -27.189 | 11.229 | 1.00 | 0.00 | 3A7 |
| ATOM | 2934 | N   | TRP | 408 | -2.334 | -25.240 | 10.202 | 1.00 | 0.00 | 3A7 |
| ATOM | 2935 | CA  | TRP | 408 | -2.553 | -24.414 | 11.368 | 1.00 | 0.00 | 3A7 |
| ATOM | 2936 | CB  | TRP | 408 | -1.243 | -23.786 | 11.891 | 1.00 | 0.00 | 3A7 |
| ATOM | 2937 | CG  | TRP | 408 | -0.242 | -24.837 | 12.291 | 1.00 | 0.00 | 3A7 |
| ATOM | 2938 | CD2 | TRP | 408 | -0.524 | -25.818 | 13.304 | 1.00 | 0.00 | 3A7 |
| ATOM | 2939 | CD1 | TRP | 408 | 1.005  | -25.107 | 11.823 | 1.00 | 0.00 | 3A7 |
| ATOM | 2940 | NE1 | TRP | 408 | 1.515  | -26.195 | 12.482 | 1.00 | 0.00 | 3A7 |
| ATOM | 2941 | CE2 | TRP | 408 | 0.574  | -26.677 | 13.353 | 1.00 | 0.00 | 3A7 |
| ATOM | 2942 | CE3 | TRP | 408 | -1.619 | -26.011 | 14.121 | 1.00 | 0.00 | 3A7 |
| ATOM | 2943 | CZ2 | TRP | 408 | 0.578  | -27.783 | 14.170 | 1.00 | 0.00 | 3A7 |
| ATOM | 2944 | CZ3 | TRP | 408 | -1.597 | -27.102 | 14.983 | 1.00 | 0.00 | 3A7 |
| ATOM | 2945 | CH2 | TRP | 408 | -0.524 | -27.989 | 14.995 | 1.00 | 0.00 | 3A7 |
| ATOM | 2946 | C   | TRP | 408 | -3.541 | -23.347 | 10.974 | 1.00 | 0.00 | 3A7 |
| ATOM | 2947 | O   | TRP | 408 | -3.197 | -22.324 | 10.383 | 1.00 | 0.00 | 3A7 |
| ATOM | 2948 | N   | THR | 409 | -4.838 | -23.556 | 11.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 2949 | CA  | THR | 409 | -5.897 | -22.587 | 11.078 | 1.00 | 0.00 | 3A7 |
| ATOM | 2950 | CB  | THR | 409 | -7.275 | -23.197 | 11.275 | 1.00 | 0.00 | 3A7 |
| ATOM | 2951 | OG1 | THR | 409 | -8.322 | -22.316 | 10.873 | 1.00 | 0.00 | 3A7 |
| ATOM | 2952 | CG2 | THR | 409 | -7.503 | -23.671 | 12.727 | 1.00 | 0.00 | 3A7 |
| ATOM | 2953 | C   | THR | 409 | -5.686 | -21.354 | 11.951 | 1.00 | 0.00 | 3A7 |
| ATOM | 2954 | O   | THR | 409 | -5.295 | -21.439 | 13.116 | 1.00 | 0.00 | 3A7 |
| ATOM | 2955 | N   | GLU | 410 | -5.888 | -20.153 | 11.363 | 1.00 | 0.00 | 3A7 |
| ATOM | 2956 | CA  | GLU | 410 | -5.519 | -18.880 | 11.957 | 1.00 | 0.00 | 3A7 |
| ATOM | 2957 | CB  | GLU | 410 | -6.432 | -18.485 | 13.138 | 1.00 | 0.00 | 3A7 |
| ATOM | 2958 | CG  | GLU | 410 | -7.920 | -18.447 | 12.751 | 1.00 | 0.00 | 3A7 |
| ATOM | 2959 | CD  | GLU | 410 | -8.744 | -18.043 | 13.970 | 1.00 | 0.00 | 3A7 |
| ATOM | 2960 | OE1 | GLU | 410 | -8.705 | -18.790 | 14.985 | 1.00 | 0.00 | 3A7 |
| ATOM | 2961 | OE2 | GLU | 410 | -9.423 | -16.984 | 13.903 | 1.00 | 0.00 | 3A7 |
| ATOM | 2962 | C   | GLU | 410 | -4.059 | -18.872 | 12.399 | 1.00 | 0.00 | 3A7 |
| ATOM | 2963 | O   | GLU | 410 | -3.756 | -18.654 | 13.572 | 1.00 | 0.00 | 3A7 |
| ATOM | 2964 | N   | PRO | 411 | -3.140 | -19.188 | 11.476 | 1.00 | 0.00 | 3A7 |
| ATOM | 2965 | CA  | PRO | 411 | -1.722 | -19.438 | 11.747 | 1.00 | 0.00 | 3A7 |
| ATOM | 2966 | CD  | PRO | 411 | -3.394 | -19.045 | 10.041 | 1.00 | 0.00 | 3A7 |
| ATOM | 2967 | CB  | PRO | 411 | -1.144 | -19.794 | 10.370 | 1.00 | 0.00 | 3A7 |
| ATOM | 2968 | CG  | PRO | 411 | -2.020 | -19.039 | 9.368  | 1.00 | 0.00 | 3A7 |
| ATOM | 2969 | C   | PRO | 411 | -1.022 | -18.216 | 12.290 | 1.00 | 0.00 | 3A7 |
| ATOM | 2970 | O   | PRO | 411 | 0.020  | -18.335 | 12.931 | 1.00 | 0.00 | 3A7 |
| ATOM | 2971 | N   | GLU | 412 | -1.592 | -17.019 | 12.058 | 1.00 | 0.00 | 3A7 |
| ATOM | 2972 | CA  | GLU | 412 | -1.018 | -15.791 | 12.493 | 1.00 | 0.00 | 3A7 |
| ATOM | 2973 | CB  | GLU | 412 | -1.368 | -14.650 | 11.516 | 1.00 | 0.00 | 3A7 |
| ATOM | 2974 | CG  | GLU | 412 | -0.914 | -14.895 | 10.063 | 1.00 | 0.00 | 3A7 |
| ATOM | 2975 | CD  | GLU | 412 | 0.609  | -14.849 | 9.920  | 1.00 | 0.00 | 3A7 |
| ATOM | 2976 | OE1 | GLU | 412 | 1.093  | -15.190 | 8.807  | 1.00 | 0.00 | 3A7 |
| ATOM | 2977 | OE2 | GLU | 412 | 1.306  | -14.468 | 10.897 | 1.00 | 0.00 | 3A7 |
| ATOM | 2978 | C   | GLU | 412 | -1.450 | -15.419 | 13.903 | 1.00 | 0.00 | 3A7 |
| ATOM | 2979 | O   | GLU | 412 | -1.079 | -14.360 | 14.405 | 1.00 | 0.00 | 3A7 |
| ATOM | 2980 | N   | LYS | 413 | -2.226 | -16.290 | 14.589 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 2981 | CA  | LYS | 413 | -2.691 | -16.035 | 15.932 | 1.00 | 0.00 | 3A7 |
| ATOM | 2982 | CB  | LYS | 413 | -4.204 | -16.281 | 16.093 | 1.00 | 0.00 | 3A7 |
| ATOM | 2983 | CG  | LYS | 413 | -5.059 | -15.300 | 15.276 | 1.00 | 0.00 | 3A7 |
| ATOM | 2984 | CD  | LYS | 413 | -6.569 | -15.457 | 15.519 | 1.00 | 0.00 | 3A7 |
| ATOM | 2985 | CE  | LYS | 413 | -7.012 | -15.075 | 16.938 | 1.00 | 0.00 | 3A7 |
| ATOM | 2986 | NZ  | LYS | 413 | -8.477 | -15.230 | 17.084 | 1.00 | 0.00 | 3A7 |
| ATOM | 2987 | C   | LYS | 413 | -1.939 | -16.896 | 16.917 | 1.00 | 0.00 | 3A7 |
| ATOM | 2988 | O   | LYS | 413 | -1.731 | -18.089 | 16.718 | 1.00 | 0.00 | 3A7 |
| ATOM | 2989 | N   | PHE | 414 | -1.550 | -16.288 | 18.059 | 1.00 | 0.00 | 3A7 |
| ATOM | 2990 | CA  | PHE | 414 | -0.981 | -16.968 | 19.200 | 1.00 | 0.00 | 3A7 |
| ATOM | 2991 | CB  | PHE | 414 | -0.298 | -15.950 | 20.125 | 1.00 | 0.00 | 3A7 |
| ATOM | 2992 | CG  | PHE | 414 | 0.563  | -16.580 | 21.179 | 1.00 | 0.00 | 3A7 |
| ATOM | 2993 | CD1 | PHE | 414 | 1.763  | -17.214 | 20.878 | 1.00 | 0.00 | 3A7 |
| ATOM | 2994 | CD2 | PHE | 414 | 0.126  | -16.541 | 22.505 | 1.00 | 0.00 | 3A7 |
| ATOM | 2995 | CE1 | PHE | 414 | 2.507  | -17.815 | 21.887 | 1.00 | 0.00 | 3A7 |
| ATOM | 2996 | CE2 | PHE | 414 | 0.864  | -17.148 | 23.513 | 1.00 | 0.00 | 3A7 |
| ATOM | 2997 | CZ  | PHE | 414 | 2.048  | -17.802 | 23.199 | 1.00 | 0.00 | 3A7 |
| ATOM | 2998 | C   | PHE | 414 | -2.045 | -17.668 | 19.981 | 1.00 | 0.00 | 3A7 |
| ATOM | 2999 | O   | PHE | 414 | -2.819 | -17.039 | 20.697 | 1.00 | 0.00 | 3A7 |
| ATOM | 3000 | N   | LEU | 415 | -2.093 | -19.006 | 19.847 | 1.00 | 0.00 | 3A7 |
| ATOM | 3001 | CA  | LEU | 415 | -3.087 | -19.816 | 20.488 | 1.00 | 0.00 | 3A7 |
| ATOM | 3002 | CB  | LEU | 415 | -4.201 | -20.254 | 19.504 | 1.00 | 0.00 | 3A7 |
| ATOM | 3003 | CG  | LEU | 415 | -5.081 | -19.105 | 18.954 | 1.00 | 0.00 | 3A7 |
| ATOM | 3004 | CD1 | LEU | 415 | -5.988 | -19.603 | 17.812 | 1.00 | 0.00 | 3A7 |
| ATOM | 3005 | CD2 | LEU | 415 | -5.911 | -18.424 | 20.058 | 1.00 | 0.00 | 3A7 |
| ATOM | 3006 | C   | LEU | 415 | -2.421 | -21.064 | 20.998 | 1.00 | 0.00 | 3A7 |
| ATOM | 3007 | O   | LEU | 415 | -2.308 | -22.038 | 20.252 | 1.00 | 0.00 | 3A7 |
| ATOM | 3008 | N   | PRO | 416 | -2.010 | -21.141 | 22.271 | 1.00 | 0.00 | 3A7 |
| ATOM | 3009 | CA  | PRO | 416 | -1.339 | -22.301 | 22.847 | 1.00 | 0.00 | 3A7 |
| ATOM | 3010 | CD  | PRO | 416 | -1.874 | -19.967 | 23.122 | 1.00 | 0.00 | 3A7 |
| ATOM | 3011 | CB  | PRO | 416 | -1.071 | -21.888 | 24.299 | 1.00 | 0.00 | 3A7 |
| ATOM | 3012 | CG  | PRO | 416 | -0.878 | -20.375 | 24.207 | 1.00 | 0.00 | 3A7 |
| ATOM | 3013 | C   | PRO | 416 | -2.201 | -23.547 | 22.780 | 1.00 | 0.00 | 3A7 |
| ATOM | 3014 | O   | PRO | 416 | -1.669 | -24.651 | 22.766 | 1.00 | 0.00 | 3A7 |
| ATOM | 3015 | N   | GLU | 417 | -3.535 | -23.381 | 22.682 | 1.00 | 0.00 | 3A7 |
| ATOM | 3016 | CA  | GLU | 417 | -4.480 | -24.458 | 22.678 | 1.00 | 0.00 | 3A7 |
| ATOM | 3017 | CB  | GLU | 417 | -5.921 | -23.933 | 22.878 | 1.00 | 0.00 | 3A7 |
| ATOM | 3018 | CG  | GLU | 417 | -6.072 | -23.126 | 24.179 | 1.00 | 0.00 | 3A7 |
| ATOM | 3019 | CD  | GLU | 417 | -7.521 | -22.672 | 24.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 3020 | OE1 | GLU | 417 | -8.172 | -23.077 | 25.322 | 1.00 | 0.00 | 3A7 |
| ATOM | 3021 | OE2 | GLU | 417 | -7.994 | -21.911 | 23.436 | 1.00 | 0.00 | 3A7 |
| ATOM | 3022 | C   | GLU | 417 | -4.459 | -25.295 | 21.427 | 1.00 | 0.00 | 3A7 |
| ATOM | 3023 | O   | GLU | 417 | -4.883 | -26.446 | 21.478 | 1.00 | 0.00 | 3A7 |
| ATOM | 3024 | N   | ARG | 418 | -3.988 | -24.733 | 20.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 3025 | CA  | ARG | 418 | -4.140 | -25.279 | 18.944 | 1.00 | 0.00 | 3A7 |
| ATOM | 3026 | CB  | ARG | 418 | -3.753 | -24.206 | 17.890 | 1.00 | 0.00 | 3A7 |
| ATOM | 3027 | CG  | ARG | 418 | -4.118 | -24.508 | 16.422 | 1.00 | 0.00 | 3A7 |
| ATOM | 3028 | CD  | ARG | 418 | -5.605 | -24.343 | 16.069 | 1.00 | 0.00 | 3A7 |
| ATOM | 3029 | NE  | ARG | 418 | -6.397 | -25.466 | 16.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 3030 | CZ  | ARG | 418 | -7.765 | -25.471 | 16.670 | 1.00 | 0.00 | 3A7 |
| ATOM | 3031 | NH1 | ARG | 418 | -8.433 | -26.503 | 17.264 | 1.00 | 0.00 | 3A7 |
| ATOM | 3032 | NH2 | ARG | 418 | -8.465 | -24.456 | 16.087 | 1.00 | 0.00 | 3A7 |
| ATOM | 3033 | C   | ARG | 418 | -3.324 | -26.538 | 18.706 | 1.00 | 0.00 | 3A7 |
| ATOM | 3034 | O   | ARG | 418 | -2.209 | -26.489 | 18.187 | 1.00 | 0.00 | 3A7 |
| ATOM | 3035 | N   | PHE | 419 | -3.919 | -27.699 | 19.103 | 1.00 | 0.00 | 3A7 |
| ATOM | 3036 | CA  | PHE | 419 | -3.457 | -29.076 | 18.984 | 1.00 | 0.00 | 3A7 |
| ATOM | 3037 | CB  | PHE | 419 | -3.390 | -29.565 | 17.516 | 1.00 | 0.00 | 3A7 |
| ATOM | 3038 | CG  | PHE | 419 | -4.772 | -29.517 | 16.915 | 1.00 | 0.00 | 3A7 |
| ATOM | 3039 | CD1 | PHE | 419 | -5.049 | -28.723 | 15.799 | 1.00 | 0.00 | 3A7 |
| ATOM | 3040 | CD2 | PHE | 419 | -5.806 | -30.278 | 17.466 | 1.00 | 0.00 | 3A7 |
| ATOM | 3041 | CE1 | PHE | 419 | -6.325 | -28.691 | 15.246 | 1.00 | 0.00 | 3A7 |
| ATOM | 3042 | CE2 | PHE | 419 | -7.085 | -30.245 | 16.919 | 1.00 | 0.00 | 3A7 |
| ATOM | 3043 | CZ  | PHE | 419 | -7.345 | -29.452 | 15.806 | 1.00 | 0.00 | 3A7 |
| ATOM | 3044 | C   | PHE | 419 | -2.135 | -29.334 | 19.681 | 1.00 | 0.00 | 3A7 |
| ATOM | 3045 | O   | PHE | 419 | -1.066 | -28.961 | 19.199 | 1.00 | 0.00 | 3A7 |
| ATOM | 3046 | N   | SER | 420 | -2.220 | -30.000 | 20.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 3047 | CA  | SER | 420 | -1.120 | -30.259 | 21.764 | 1.00 | 0.00 | 3A7 |
| ATOM | 3048 | CB  | SER | 420 | -1.589 | -30.137 | 23.241 | 1.00 | 0.00 | 3A7 |
| ATOM | 3049 | OG  | SER | 420 | -0.513 | -30.208 | 24.172 | 1.00 | 0.00 | 3A7 |
| ATOM | 3050 | C   | SER | 420 | -0.568 | -31.644 | 21.508 | 1.00 | 0.00 | 3A7 |
| ATOM | 3051 | O   | SER | 420 | -1.267 | -32.527 | 21.013 | 1.00 | 0.00 | 3A7 |
| ATOM | 3052 | N   | LYS | 421 | 0.722  | -31.842 | 21.877 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3053 | CA  | LYS | 421 | 1.404  | -33.112 | 21.813 | 1.00 | 0.00 | 3A7 |
| ATOM | 3054 | CB  | LYS | 421 | 2.506  | -33.196 | 20.717 | 1.00 | 0.00 | 3A7 |
| ATOM | 3055 | CG  | LYS | 421 | 3.804  | -32.380 | 20.921 | 1.00 | 0.00 | 3A7 |
| ATOM | 3056 | CD  | LYS | 421 | 3.679  | -30.845 | 20.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 3057 | CE  | LYS | 421 | 3.332  | -30.147 | 19.673 | 1.00 | 0.00 | 3A7 |
| ATOM | 3058 | NZ  | LYS | 421 | 1.927  | -30.385 | 19.273 | 1.00 | 0.00 | 3A7 |
| ATOM | 3059 | C   | LYS | 421 | 2.007  | -33.350 | 23.167 | 1.00 | 0.00 | 3A7 |
| ATOM | 3060 | O   | LYS | 421 | 2.165  | -32.424 | 23.962 | 1.00 | 0.00 | 3A7 |
| ATOM | 3061 | N   | LYS | 422 | 2.373  | -34.620 | 23.448 | 1.00 | 0.00 | 3A7 |
| ATOM | 3062 | CA  | LYS | 422 | 3.032  | -34.986 | 24.675 | 1.00 | 0.00 | 3A7 |
| ATOM | 3063 | CB  | LYS | 422 | 2.048  | -35.203 | 25.856 | 1.00 | 0.00 | 3A7 |
| ATOM | 3064 | CG  | LYS | 422 | 2.715  | -35.433 | 27.225 | 1.00 | 0.00 | 3A7 |
| ATOM | 3065 | CD  | LYS | 422 | 3.520  | -34.222 | 27.727 | 1.00 | 0.00 | 3A7 |
| ATOM | 3066 | CE  | LYS | 422 | 4.151  | -34.436 | 29.109 | 1.00 | 0.00 | 3A7 |
| ATOM | 3067 | NZ  | LYS | 422 | 5.140  | -35.537 | 29.071 | 1.00 | 0.00 | 3A7 |
| ATOM | 3068 | C   | LYS | 422 | 3.767  | -36.262 | 24.379 | 1.00 | 0.00 | 3A7 |
| ATOM | 3069 | O   | LYS | 422 | 4.874  | -36.483 | 24.867 | 1.00 | 0.00 | 3A7 |
| ATOM | 3070 | N   | ASN | 423 | 3.138  | -37.137 | 23.555 | 1.00 | 0.00 | 3A7 |
| ATOM | 3071 | CA  | ASN | 423 | 3.658  | -38.427 | 23.165 | 1.00 | 0.00 | 3A7 |
| ATOM | 3072 | CB  | ASN | 423 | 2.646  | -39.581 | 23.442 | 1.00 | 0.00 | 3A7 |
| ATOM | 3073 | CG  | ASN | 423 | 1.264  | -39.329 | 22.812 | 1.00 | 0.00 | 3A7 |
| ATOM | 3074 | OD1 | ASN | 423 | 0.498  | -38.476 | 23.277 | 1.00 | 0.00 | 3A7 |
| ATOM | 3075 | ND2 | ASN | 423 | 0.950  | -40.110 | 21.734 | 1.00 | 0.00 | 3A7 |
| ATOM | 3076 | C   | ASN | 423 | 4.031  | -38.367 | 21.703 | 1.00 | 0.00 | 3A7 |
| ATOM | 3077 | O   | ASN | 423 | 3.916  | -37.323 | 21.061 | 1.00 | 0.00 | 3A7 |
| ATOM | 3078 | N   | LYS | 424 | 4.481  | -39.522 | 21.148 | 1.00 | 0.00 | 3A7 |
| ATOM | 3079 | CA  | LYS | 424 | 4.861  | -39.684 | 19.760 | 1.00 | 0.00 | 3A7 |
| ATOM | 3080 | CB  | LYS | 424 | 5.998  | -40.724 | 19.591 | 1.00 | 0.00 | 3A7 |
| ATOM | 3081 | CG  | LYS | 424 | 6.530  | -40.859 | 18.153 | 1.00 | 0.00 | 3A7 |
| ATOM | 3082 | CD  | LYS | 424 | 7.676  | -41.874 | 18.013 | 1.00 | 0.00 | 3A7 |
| ATOM | 3083 | CE  | LYS | 424 | 8.960  | -41.460 | 18.744 | 1.00 | 0.00 | 3A7 |
| ATOM | 3084 | NZ  | LYS | 424 | 10.027 | -42.465 | 18.534 | 1.00 | 0.00 | 3A7 |
| ATOM | 3085 | C   | LYS | 424 | 3.649  | -40.125 | 18.981 | 1.00 | 0.00 | 3A7 |
| ATOM | 3086 | O   | LYS | 424 | 3.011  | -41.116 | 19.335 | 1.00 | 0.00 | 3A7 |
| ATOM | 3087 | N   | ASP | 425 | 3.321  | -39.353 | 17.910 | 1.00 | 0.00 | 3A7 |
| ATOM | 3088 | CA  | ASP | 425 | 2.171  | -39.492 | 17.032 | 1.00 | 0.00 | 3A7 |
| ATOM | 3089 | CB  | ASP | 425 | 1.794  | -40.959 | 16.658 | 1.00 | 0.00 | 3A7 |
| ATOM | 3090 | CG  | ASP | 425 | 0.795  | -41.005 | 15.496 | 1.00 | 0.00 | 3A7 |
| ATOM | 3091 | OD1 | ASP | 425 | -0.322 | -41.550 | 15.698 | 1.00 | 0.00 | 3A7 |
| ATOM | 3092 | OD2 | ASP | 425 | 1.142  | -40.497 | 14.397 | 1.00 | 0.00 | 3A7 |
| ATOM | 3093 | C   | ASP | 425 | 1.009  | -38.771 | 17.679 | 1.00 | 0.00 | 3A7 |
| ATOM | 3094 | O   | ASP | 425 | 0.241  | -39.355 | 18.444 | 1.00 | 0.00 | 3A7 |
| ATOM | 3095 | N   | ASN | 426 | 0.881  | -37.457 | 17.372 | 1.00 | 0.00 | 3A7 |
| ATOM | 3096 | CA  | ASN | 426 | -0.110 | -36.573 | 17.945 | 1.00 | 0.00 | 3A7 |
| ATOM | 3097 | CB  | ASN | 426 | 0.515  | -35.250 | 18.487 | 1.00 | 0.00 | 3A7 |
| ATOM | 3098 | CG  | ASN | 426 | 1.320  | -34.458 | 17.438 | 1.00 | 0.00 | 3A7 |
| ATOM | 3099 | OD1 | ASN | 426 | 2.282  | -34.963 | 16.848 | 1.00 | 0.00 | 3A7 |
| ATOM | 3100 | ND2 | ASN | 426 | 0.912  | -33.168 | 17.234 | 1.00 | 0.00 | 3A7 |
| ATOM | 3101 | C   | ASN | 426 | -1.189 | -36.329 | 16.915 | 1.00 | 0.00 | 3A7 |
| ATOM | 3102 | O   | ASN | 426 | -1.547 | -37.229 | 16.157 | 1.00 | 0.00 | 3A7 |
| ATOM | 3103 | N   | ILE | 427 | -1.746 | -35.090 | 16.880 | 1.00 | 0.00 | 3A7 |
| ATOM | 3104 | CA  | ILE | 427 | -2.849 | -34.709 | 16.022 | 1.00 | 0.00 | 3A7 |
| ATOM | 3105 | CB  | ILE | 427 | -3.731 | -33.632 | 16.647 | 1.00 | 0.00 | 3A7 |
| ATOM | 3106 | CG2 | ILE | 427 | -4.975 | -33.389 | 15.762 | 1.00 | 0.00 | 3A7 |
| ATOM | 3107 | CG1 | ILE | 427 | -4.130 | -34.009 | 18.097 | 1.00 | 0.00 | 3A7 |
| ATOM | 3108 | CD  | ILE | 427 | -4.944 | -35.302 | 18.218 | 1.00 | 0.00 | 3A7 |
| ATOM | 3109 | C   | ILE | 427 | -2.306 | -34.224 | 14.699 | 1.00 | 0.00 | 3A7 |
| ATOM | 3110 | O   | ILE | 427 | -2.782 | -34.635 | 13.641 | 1.00 | 0.00 | 3A7 |
| ATOM | 3111 | N   | ASP | 428 | -1.289 | -33.326 | 14.741 | 1.00 | 0.00 | 3A7 |
| ATOM | 3112 | CA  | ASP | 428 | -0.691 | -32.752 | 13.555 | 1.00 | 0.00 | 3A7 |
| ATOM | 3113 | CB  | ASP | 428 | -1.067 | -31.262 | 13.360 | 1.00 | 0.00 | 3A7 |
| ATOM | 3114 | CG  | ASP | 428 | -2.578 | -31.131 | 13.173 | 1.00 | 0.00 | 3A7 |
| ATOM | 3115 | OD1 | ASP | 428 | -3.101 | -31.683 | 12.169 | 1.00 | 0.00 | 3A7 |
| ATOM | 3116 | OD2 | ASP | 428 | -3.224 | -30.473 | 14.030 | 1.00 | 0.00 | 3A7 |
| ATOM | 3117 | C   | ASP | 428 | 0.815  | -32.877 | 13.650 | 1.00 | 0.00 | 3A7 |
| ATOM | 3118 | O   | ASP | 428 | 1.471  | -31.935 | 14.093 | 1.00 | 0.00 | 3A7 |
| ATOM | 3119 | N   | PRO | 429 | 1.414  | -34.003 | 13.251 | 1.00 | 0.00 | 3A7 |
| ATOM | 3120 | CA  | PRO | 429 | 2.856  | -34.177 | 13.157 | 1.00 | 0.00 | 3A7 |
| ATOM | 3121 | CD  | PRO | 429 | 0.694  | -35.245 | 12.998 | 1.00 | 0.00 | 3A7 |
| ATOM | 3122 | CB  | PRO | 429 | 3.026  | -35.701 | 13.258 | 1.00 | 0.00 | 3A7 |
| ATOM | 3123 | CG  | PRO | 429 | 1.763  | -36.266 | 12.604 | 1.00 | 0.00 | 3A7 |
| ATOM | 3124 | C   | PRO | 429 | 3.490  | -33.658 | 11.858 | 1.00 | 0.00 | 3A7 |



|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3125 | O   | PRO | 429 | 2.892  | -33.616 | 10.780 | 1.00 | 0.00 | 3A7 |
| ATOM | 3126 | N   | TYR | 430 | 4.793  | -33.325 | 11.967 | 1.00 | 0.00 | 3A7 |
| ATOM | 3127 | CA  | TYR | 430 | 5.745  | -33.153 | 10.884 | 1.00 | 0.00 | 3A7 |
| ATOM | 3128 | CB  | TYR | 430 | 5.621  | -34.248 | 9.770  | 1.00 | 0.00 | 3A7 |
| ATOM | 3129 | CG  | TYR | 430 | 6.889  | -34.285 | 8.969  | 1.00 | 0.00 | 3A7 |
| ATOM | 3130 | CD1 | TYR | 430 | 8.048  | -34.836 | 9.516  | 1.00 | 0.00 | 3A7 |
| ATOM | 3131 | CD2 | TYR | 430 | 6.967  | -33.566 | 7.779  | 1.00 | 0.00 | 3A7 |
| ATOM | 3132 | CE1 | TYR | 430 | 9.284  | -34.596 | 8.926  | 1.00 | 0.00 | 3A7 |
| ATOM | 3133 | CE2 | TYR | 430 | 8.205  | -33.267 | 7.232  | 1.00 | 0.00 | 3A7 |
| ATOM | 3134 | CZ  | TYR | 430 | 9.366  | -33.774 | 7.806  | 1.00 | 0.00 | 3A7 |
| ATOM | 3135 | OH  | TYR | 430 | 10.620 | -33.421 | 7.266  | 1.00 | 0.00 | 3A7 |
| ATOM | 3136 | C   | TYR | 430 | 5.763  | -31.761 | 10.274 | 1.00 | 0.00 | 3A7 |
| ATOM | 3137 | O   | TYR | 430 | 6.683  | -31.428 | 9.529  | 1.00 | 0.00 | 3A7 |
| ATOM | 3138 | N   | ILE | 431 | 4.795  | -30.877 | 10.599 | 1.00 | 0.00 | 3A7 |
| ATOM | 3139 | CA  | ILE | 431 | 4.842  | -29.502 | 10.146 | 1.00 | 0.00 | 3A7 |
| ATOM | 3140 | CB  | ILE | 431 | 3.495  | -28.893 | 9.784  | 1.00 | 0.00 | 3A7 |
| ATOM | 3141 | CG2 | ILE | 431 | 2.954  | -29.661 | 8.570  | 1.00 | 0.00 | 3A7 |
| ATOM | 3142 | CG1 | ILE | 431 | 2.477  | -28.800 | 10.949 | 1.00 | 0.00 | 3A7 |
| ATOM | 3143 | CD  | ILE | 431 | 1.966  | -30.124 | 11.513 | 1.00 | 0.00 | 3A7 |
| ATOM | 3144 | C   | ILE | 431 | 5.480  | -28.630 | 11.193 | 1.00 | 0.00 | 3A7 |
| ATOM | 3145 | O   | ILE | 431 | 5.889  | -27.509 | 10.893 | 1.00 | 0.00 | 3A7 |
| ATOM | 3146 | N   | TYR | 432 | 5.562  | -29.122 | 12.460 | 1.00 | 0.00 | 3A7 |
| ATOM | 3147 | CA  | TYR | 432 | 6.198  | -28.443 | 13.571 | 1.00 | 0.00 | 3A7 |
| ATOM | 3148 | CB  | TYR | 432 | 5.758  | -28.969 | 14.973 | 1.00 | 0.00 | 3A7 |
| ATOM | 3149 | CG  | TYR | 432 | 4.498  | -28.367 | 15.505 | 1.00 | 0.00 | 3A7 |
| ATOM | 3150 | CD1 | TYR | 432 | 3.438  | -29.190 | 15.886 | 1.00 | 0.00 | 3A7 |
| ATOM | 3151 | CD2 | TYR | 432 | 4.439  | -27.004 | 15.799 | 1.00 | 0.00 | 3A7 |
| ATOM | 3152 | CE1 | TYR | 432 | 2.350  | -28.665 | 16.575 | 1.00 | 0.00 | 3A7 |
| ATOM | 3153 | CE2 | TYR | 432 | 3.348  | -26.477 | 16.484 | 1.00 | 0.00 | 3A7 |
| ATOM | 3154 | CZ  | TYR | 432 | 2.304  | -27.307 | 16.878 | 1.00 | 0.00 | 3A7 |
| ATOM | 3155 | OH  | TYR | 432 | 1.204  | -26.773 | 17.586 | 1.00 | 0.00 | 3A7 |
| ATOM | 3156 | C   | TYR | 432 | 7.676  | -28.741 | 13.531 | 1.00 | 0.00 | 3A7 |
| ATOM | 3157 | O   | TYR | 432 | 8.161  | -29.675 | 14.169 | 1.00 | 0.00 | 3A7 |
| ATOM | 3158 | N   | THR | 433 | 8.425  | -27.919 | 12.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 3159 | CA  | THR | 433 | 9.824  | -28.119 | 12.506 | 1.00 | 0.00 | 3A7 |
| ATOM | 3160 | CB  | THR | 433 | 10.074 | -28.167 | 10.995 | 1.00 | 0.00 | 3A7 |
| ATOM | 3161 | OG1 | THR | 433 | 9.638  | -26.980 | 10.336 | 1.00 | 0.00 | 3A7 |
| ATOM | 3162 | CG2 | THR | 433 | 9.309  | -29.368 | 10.401 | 1.00 | 0.00 | 3A7 |
| ATOM | 3163 | C   | THR | 433 | 10.729 | -27.070 | 13.107 | 1.00 | 0.00 | 3A7 |
| ATOM | 3164 | O   | THR | 433 | 11.720 | -26.744 | 12.459 | 1.00 | 0.00 | 3A7 |
| ATOM | 3165 | N   | PRO | 434 | 10.544 | -26.494 | 14.305 | 1.00 | 0.00 | 3A7 |
| ATOM | 3166 | CA  | PRO | 434 | 11.476 | -25.526 | 14.854 | 1.00 | 0.00 | 3A7 |
| ATOM | 3167 | CD  | PRO | 434 | 9.603  | -26.944 | 15.329 | 1.00 | 0.00 | 3A7 |
| ATOM | 3168 | CB  | PRO | 434 | 10.738 | -25.003 | 16.098 | 1.00 | 0.00 | 3A7 |
| ATOM | 3169 | CG  | PRO | 434 | 9.981  | -26.220 | 16.622 | 1.00 | 0.00 | 3A7 |
| ATOM | 3170 | C   | PRO | 434 | 12.807 | -26.180 | 15.226 | 1.00 | 0.00 | 3A7 |
| ATOM | 3171 | O   | PRO | 434 | 13.809 | -25.477 | 15.300 | 1.00 | 0.00 | 3A7 |
| ATOM | 3172 | N   | PHE | 435 | 12.847 | -27.518 | 15.456 | 1.00 | 0.00 | 3A7 |
| ATOM | 3173 | CA  | PHE | 435 | 14.041 | -28.253 | 15.844 | 1.00 | 0.00 | 3A7 |
| ATOM | 3174 | CB  | PHE | 435 | 13.670 | -29.173 | 17.045 | 1.00 | 0.00 | 3A7 |
| ATOM | 3175 | CG  | PHE | 435 | 13.744 | -28.509 | 18.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 3176 | CD1 | PHE | 435 | 14.729 | -27.557 | 18.520 | 1.00 | 0.00 | 3A7 |
| ATOM | 3177 | CD2 | PHE | 435 | 12.731 | -28.261 | 19.269 | 1.00 | 0.00 | 3A7 |
| ATOM | 3178 | CE1 | PHE | 435 | 14.264 | -26.403 | 19.460 | 1.00 | 0.00 | 3A7 |
| ATOM | 3179 | CE2 | PHE | 435 | 14.105 | -27.600 | 20.460 | 1.00 | 0.00 | 3A7 |
| ATOM | 3180 | CZ  | PHE | 435 | 13.408 | -26.726 | 20.695 | 1.00 | 0.00 | 3A7 |
| ATOM | 3181 | C   | PHE | 435 | 14.509 | -29.099 | 14.689 | 1.00 | 0.00 | 3A7 |
| ATOM | 3182 | O   | PHE | 435 | 15.352 | -29.980 | 14.855 | 1.00 | 0.00 | 3A7 |
| ATOM | 3183 | N   | GLY | 436 | 13.993 | -28.834 | 13.469 | 1.00 | 0.00 | 3A7 |
| ATOM | 3184 | CA  | GLY | 436 | 14.463 | -29.495 | 12.269 | 1.00 | 0.00 | 3A7 |
| ATOM | 3185 | C   | GLY | 436 | 13.733 | -30.777 | 12.129 | 1.00 | 0.00 | 3A7 |
| ATOM | 3186 | O   | GLY | 436 | 12.792 | -31.061 | 12.870 | 1.00 | 0.00 | 3A7 |
| ATOM | 3187 | N   | SER | 437 | 14.147 | -31.599 | 11.152 | 1.00 | 0.00 | 3A7 |
| ATOM | 3188 | CA  | SER | 437 | 13.525 | -32.872 | 10.944 | 1.00 | 0.00 | 3A7 |
| ATOM | 3189 | CB  | SER | 437 | 12.322 | -32.829 | 9.974  | 1.00 | 0.00 | 3A7 |
| ATOM | 3190 | OG  | SER | 437 | 11.247 | -32.079 | 10.518 | 1.00 | 0.00 | 3A7 |
| ATOM | 3191 | C   | SER | 437 | 14.585 | -33.730 | 10.351 | 1.00 | 0.00 | 3A7 |
| ATOM | 3192 | O   | SER | 437 | 15.352 | -33.291 | 9.494  | 1.00 | 0.00 | 3A7 |
| ATOM | 3193 | N   | GLY | 438 | 14.623 | -35.006 | 10.788 | 1.00 | 0.00 | 3A7 |
| ATOM | 3194 | CA  | GLY | 438 | 15.462 | -36.010 | 10.184 | 1.00 | 0.00 | 3A7 |
| ATOM | 3195 | C   | GLY | 438 | 16.610 | -36.414 | 11.067 | 1.00 | 0.00 | 3A7 |
| ATOM | 3196 | O   | GLY | 438 | 16.526 | -36.346 | 12.293 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3197 | N   | PRO | 439 | 17.704 | -36.873 | 10.443 | 1.00 | 0.00 | 3A7 |
| ATOM | 3198 | CA  | PRO | 439 | 18.897 | -37.275 | 11.180 | 1.00 | 0.00 | 3A7 |
| ATOM | 3199 | CD  | PRO | 439 | 17.653 | -37.555 | 9.152  | 1.00 | 0.00 | 3A7 |
| ATOM | 3200 | CB  | PRO | 439 | 19.741 | -38.079 | 10.170 | 1.00 | 0.00 | 3A7 |
| ATOM | 3201 | CG  | PRO | 439 | 18.702 | -38.666 | 9.220  | 1.00 | 0.00 | 3A7 |
| ATOM | 3202 | C   | PRO | 439 | 19.700 | -36.119 | 11.729 | 1.00 | 0.00 | 3A7 |
| ATOM | 3203 | O   | PRO | 439 | 20.523 | -36.342 | 12.614 | 1.00 | 0.00 | 3A7 |
| ATOM | 3204 | N   | ARG | 440 | 19.490 | -34.889 | 11.217 | 1.00 | 0.00 | 3A7 |
| ATOM | 3205 | CA  | ARG | 440 | 20.212 | -33.720 | 11.642 | 1.00 | 0.00 | 3A7 |
| ATOM | 3206 | CB  | ARG | 440 | 20.704 | -32.913 | 10.433 | 1.00 | 0.00 | 3A7 |
| ATOM | 3207 | CG  | ARG | 440 | 21.775 | -33.662 | 9.617  | 1.00 | 0.00 | 3A7 |
| ATOM | 3208 | CD  | ARG | 440 | 21.846 | -33.224 | 8.148  | 1.00 | 0.00 | 3A7 |
| ATOM | 3209 | NE  | ARG | 440 | 20.618 | -33.741 | 7.458  | 1.00 | 0.00 | 3A7 |
| ATOM | 3210 | CZ  | ARG | 440 | 20.391 | -33.552 | 6.123  | 1.00 | 0.00 | 3A7 |
| ATOM | 3211 | NH1 | ARG | 440 | 19.299 | -34.126 | 5.537  | 1.00 | 0.00 | 3A7 |
| ATOM | 3212 | NH2 | ARG | 440 | 21.244 | -32.799 | 5.371  | 1.00 | 0.00 | 3A7 |
| ATOM | 3213 | C   | ARG | 440 | 19.307 | -32.855 | 12.480 | 1.00 | 0.00 | 3A7 |
| ATOM | 3214 | O   | ARG | 440 | 19.471 | -31.639 | 12.565 | 1.00 | 0.00 | 3A7 |
| ATOM | 3215 | N   | ASN | 441 | 18.322 | -33.480 | 13.163 | 1.00 | 0.00 | 3A7 |
| ATOM | 3216 | CA  | ASN | 441 | 17.420 | -32.809 | 14.066 | 1.00 | 0.00 | 3A7 |
| ATOM | 3217 | CB  | ASN | 441 | 16.263 | -33.734 | 14.515 | 1.00 | 0.00 | 3A7 |
| ATOM | 3218 | CG  | ASN | 441 | 16.713 | -34.970 | 15.324 | 1.00 | 0.00 | 3A7 |
| ATOM | 3219 | OD1 | ASN | 441 | 17.527 | -35.781 | 14.869 | 1.00 | 0.00 | 3A7 |
| ATOM | 3220 | ND2 | ASN | 441 | 16.154 | -35.093 | 16.567 | 1.00 | 0.00 | 3A7 |
| ATOM | 3221 | C   | ASN | 441 | 18.197 | -32.339 | 15.260 | 1.00 | 0.00 | 3A7 |
| ATOM | 3222 | O   | ASN | 441 | 19.263 | -32.884 | 15.550 | 1.00 | 0.00 | 3A7 |
| ATOM | 3223 | N   | CYS | 442 | 17.690 | -31.324 | 15.990 | 1.00 | 0.00 | 3A7 |
| ATOM | 3224 | CA  | CYS | 442 | 18.409 | -30.739 | 17.097 | 1.00 | 0.00 | 3A7 |
| ATOM | 3225 | CB  | CYS | 442 | 17.629 | -29.548 | 17.676 | 1.00 | 0.00 | 3A7 |
| ATOM | 3226 | SG  | CYS | 442 | 18.592 | -28.606 | 18.905 | 1.00 | 0.00 | 3A7 |
| ATOM | 3227 | C   | CYS | 442 | 18.683 | -31.758 | 18.181 | 1.00 | 0.00 | 3A7 |
| ATOM | 3228 | O   | CYS | 442 | 17.779 | -32.410 | 18.699 | 1.00 | 0.00 | 3A7 |
| ATOM | 3229 | N   | ILE | 443 | 19.971 | -31.894 | 18.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 3230 | CA  | ILE | 443 | 20.405 | -32.830 | 19.531 | 1.00 | 0.00 | 3A7 |
| ATOM | 3231 | CB  | ILE | 443 | 21.872 | -33.211 | 19.324 | 1.00 | 0.00 | 3A7 |
| ATOM | 3232 | CG2 | ILE | 443 | 22.414 | -34.095 | 20.472 | 1.00 | 0.00 | 3A7 |
| ATOM | 3233 | CG1 | ILE | 443 | 22.046 | -33.916 | 17.955 | 1.00 | 0.00 | 3A7 |
| ATOM | 3234 | CD  | ILE | 443 | 21.378 | -35.291 | 17.849 | 1.00 | 0.00 | 3A7 |
| ATOM | 3235 | C   | ILE | 443 | 20.167 | -32.223 | 20.902 | 1.00 | 0.00 | 3A7 |
| ATOM | 3236 | O   | ILE | 443 | 20.008 | -32.929 | 21.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 3237 | N   | GLY | 444 | 20.106 | -30.876 | 20.975 | 1.00 | 0.00 | 3A7 |
| ATOM | 3238 | CA  | GLY | 444 | 19.894 | -30.159 | 22.204 | 1.00 | 0.00 | 3A7 |
| ATOM | 3239 | C   | GLY | 444 | 18.471 | -29.893 | 22.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 3240 | O   | GLY | 444 | 18.222 | -29.153 | 23.479 | 1.00 | 0.00 | 3A7 |
| ATOM | 3241 | N   | MET | 445 | 17.493 | -30.471 | 21.788 | 1.00 | 0.00 | 3A7 |
| ATOM | 3242 | CA  | MET | 445 | 16.056 | -30.254 | 21.939 | 1.00 | 0.00 | 3A7 |
| ATOM | 3243 | CB  | MET | 445 | 15.279 | -31.201 | 21.002 | 1.00 | 0.00 | 3A7 |
| ATOM | 3244 | CG  | MET | 445 | 13.742 | -31.222 | 21.137 | 1.00 | 0.00 | 3A7 |
| ATOM | 3245 | SD  | MET | 445 | 12.898 | -32.098 | 19.780 | 1.00 | 0.00 | 3A7 |
| ATOM | 3246 | CE  | MET | 445 | 13.584 | -33.749 | 20.107 | 1.00 | 0.00 | 3A7 |
| ATOM | 3247 | C   | MET | 445 | 15.558 | -30.454 | 23.349 | 1.00 | 0.00 | 3A7 |
| ATOM | 3248 | O   | MET | 445 | 14.887 | -29.598 | 23.919 | 1.00 | 0.00 | 3A7 |
| ATOM | 3249 | N   | ARG | 446 | 15.928 | -31.580 | 23.976 | 1.00 | 0.00 | 3A7 |
| ATOM | 3250 | CA  | ARG | 446 | 15.476 | -31.910 | 25.309 | 1.00 | 0.00 | 3A7 |
| ATOM | 3251 | CB  | ARG | 446 | 15.826 | -33.368 | 25.684 | 1.00 | 0.00 | 3A7 |
| ATOM | 3252 | CG  | ARG | 446 | 15.490 | -34.340 | 24.538 | 1.00 | 0.00 | 3A7 |
| ATOM | 3253 | CD  | ARG | 446 | 15.588 | -35.824 | 24.911 | 1.00 | 0.00 | 3A7 |
| ATOM | 3254 | NE  | ARG | 446 | 14.428 | -36.164 | 25.799 | 1.00 | 0.00 | 3A7 |
| ATOM | 3255 | CZ  | ARG | 446 | 14.005 | -37.451 | 25.986 | 1.00 | 0.00 | 3A7 |
| ATOM | 3256 | NH1 | ARG | 446 | 12.921 | -37.696 | 26.780 | 1.00 | 0.00 | 3A7 |
| ATOM | 3257 | NH2 | ARG | 446 | 14.658 | -38.492 | 25.394 | 1.00 | 0.00 | 3A7 |
| ATOM | 3258 | C   | ARG | 446 | 16.001 | -30.952 | 26.348 | 1.00 | 0.00 | 3A7 |
| ATOM | 3259 | O   | ARG | 446 | 15.276 | -30.542 | 27.248 | 1.00 | 0.00 | 3A7 |
| ATOM | 3260 | N   | PHE | 447 | 17.267 | -30.512 | 26.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 3261 | CA  | PHE | 447 | 17.865 | -29.566 | 27.113 | 1.00 | 0.00 | 3A7 |
| ATOM | 3262 | CB  | PHE | 447 | 19.408 | -29.515 | 27.061 | 1.00 | 0.00 | 3A7 |
| ATOM | 3263 | CG  | PHE | 447 | 19.952 | -30.827 | 26.613 | 1.00 | 0.00 | 3A7 |
| ATOM | 3264 | CD1 | PHE | 447 | 20.810 | -30.828 | 25.520 | 1.00 | 0.00 | 3A7 |
| ATOM | 3265 | CD2 | PHE | 447 | 19.433 | -32.037 | 27.086 | 1.00 | 0.00 | 3A7 |
| ATOM | 3266 | CE1 | PHE | 447 | 20.971 | -31.985 | 24.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 3267 | CE2 | PHE | 447 | 19.526 | -33.173 | 26.291 | 1.00 | 0.00 | 3A7 |
| ATOM | 3268 | CZ  | PHE | 447 | 20.229 | -33.109 | 25.096 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3269 | C   | PHE | 447 | 17.285 | -28.185 | 26.918 | 1.00 | 0.00 | 3A7 |
| ATOM | 3270 | O   | PHE | 447 | 17.071 | -27.458 | 27.881 | 1.00 | 0.00 | 3A7 |
| ATOM | 3271 | N   | ALA | 448 | 16.949 | -27.798 | 25.656 | 1.00 | 0.00 | 3A7 |
| ATOM | 3272 | CA  | ALA | 448 | 16.406 | -26.493 | 25.374 | 1.00 | 0.00 | 3A7 |
| ATOM | 3273 | CB  | ALA | 448 | 16.379 | -26.216 | 23.882 | 1.00 | 0.00 | 3A7 |
| ATOM | 3274 | C   | ALA | 448 | 15.020 | -26.344 | 25.914 | 1.00 | 0.00 | 3A7 |
| ATOM | 3275 | O   | ALA | 448 | 14.679 | -25.313 | 26.493 | 1.00 | 0.00 | 3A7 |
| ATOM | 3276 | N   | LEU | 449 | 14.197 | -27.406 | 25.800 | 1.00 | 0.00 | 3A7 |
| ATOM | 3277 | CA  | LEU | 449 | 12.842 | -27.402 | 26.309 | 1.00 | 0.00 | 3A7 |
| ATOM | 3278 | CB  | LEU | 449 | 12.029 | -28.605 | 25.813 | 1.00 | 0.00 | 3A7 |
| ATOM | 3279 | CG  | LEU | 449 | 11.639 | -28.523 | 24.324 | 1.00 | 0.00 | 3A7 |
| ATOM | 3280 | CD1 | LEU | 449 | 11.120 | -29.879 | 23.807 | 1.00 | 0.00 | 3A7 |
| ATOM | 3281 | CD2 | LEU | 449 | 10.621 | -27.401 | 24.038 | 1.00 | 0.00 | 3A7 |
| ATOM | 3282 | C   | LEU | 449 | 12.800 | -27.422 | 27.811 | 1.00 | 0.00 | 3A7 |
| ATOM | 3283 | O   | LEU | 449 | 11.936 | -26.797 | 28.417 | 1.00 | 0.00 | 3A7 |
| ATOM | 3284 | N   | VAL | 450 | 13.770 | -28.111 | 28.454 | 1.00 | 0.00 | 3A7 |
| ATOM | 3285 | CA  | VAL | 450 | 13.883 | -28.171 | 29.893 | 1.00 | 0.00 | 3A7 |
| ATOM | 3286 | CB  | VAL | 450 | 14.890 | -29.213 | 30.345 | 1.00 | 0.00 | 3A7 |
| ATOM | 3287 | CG1 | VAL | 450 | 15.177 | -29.141 | 31.862 | 1.00 | 0.00 | 3A7 |
| ATOM | 3288 | CG2 | VAL | 450 | 14.262 | -30.592 | 30.049 | 1.00 | 0.00 | 3A7 |
| ATOM | 3289 | C   | VAL | 450 | 14.256 | -26.828 | 30.431 | 1.00 | 0.00 | 3A7 |
| ATOM | 3290 | O   | VAL | 450 | 13.633 | -26.345 | 31.364 | 1.00 | 0.00 | 3A7 |
| ATOM | 3291 | N   | ASN | 451 | 15.263 | -26.162 | 29.833 | 1.00 | 0.00 | 3A7 |
| ATOM | 3292 | CA  | ASN | 451 | 15.735 | -24.855 | 30.232 | 1.00 | 0.00 | 3A7 |
| ATOM | 3293 | CB  | ASN | 451 | 16.873 | -24.401 | 29.295 | 1.00 | 0.00 | 3A7 |
| ATOM | 3294 | CG  | ASN | 451 | 18.141 | -25.243 | 29.476 | 1.00 | 0.00 | 3A7 |
| ATOM | 3295 | OD1 | ASN | 451 | 18.233 | -26.089 | 30.369 | 1.00 | 0.00 | 3A7 |
| ATOM | 3296 | ND2 | ASN | 451 | 19.145 | -24.981 | 28.583 | 1.00 | 0.00 | 3A7 |
| ATOM | 3297 | C   | ASN | 451 | 14.659 | -23.792 | 30.150 | 1.00 | 0.00 | 3A7 |
| ATOM | 3298 | O   | ASN | 451 | 14.440 | -23.023 | 31.081 | 1.00 | 0.00 | 3A7 |
| ATOM | 3299 | N   | MET | 452 | 13.918 | -23.759 | 29.019 | 1.00 | 0.00 | 3A7 |
| ATOM | 3300 | CA  | MET | 452 | 12.853 | -22.808 | 28.800 | 1.00 | 0.00 | 3A7 |
| ATOM | 3301 | CB  | MET | 452 | 12.311 | -22.880 | 27.353 | 1.00 | 0.00 | 3A7 |
| ATOM | 3302 | CG  | MET | 452 | 13.202 | -22.090 | 26.370 | 1.00 | 0.00 | 3A7 |
| ATOM | 3303 | SD  | MET | 452 | 13.800 | -22.975 | 24.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 3304 | CE  | MET | 452 | 12.280 | -23.810 | 24.359 | 1.00 | 0.00 | 3A7 |
| ATOM | 3305 | C   | MET | 452 | 11.733 | -22.982 | 29.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 3306 | O   | MET | 452 | 11.255 | -22.013 | 30.355 | 1.00 | 0.00 | 3A7 |
| ATOM | 3307 | N   | LYS | 453 | 11.310 | -24.236 | 30.042 | 1.00 | 0.00 | 3A7 |
| ATOM | 3308 | CA  | LYS | 453 | 10.240 | -24.536 | 30.965 | 1.00 | 0.00 | 3A7 |
| ATOM | 3309 | CB  | LYS | 453 | 9.864  | -26.021 | 30.868 | 1.00 | 0.00 | 3A7 |
| ATOM | 3310 | CG  | LYS | 453 | 8.486  | -26.409 | 31.399 | 1.00 | 0.00 | 3A7 |
| ATOM | 3311 | CD  | LYS | 453 | 8.218  | -27.911 | 31.258 | 1.00 | 0.00 | 3A7 |
| ATOM | 3312 | CE  | LYS | 453 | 8.280  | -28.457 | 29.817 | 1.00 | 0.00 | 3A7 |
| ATOM | 3313 | NZ  | LYS | 453 | 9.661  | -28.675 | 29.322 | 1.00 | 0.00 | 3A7 |
| ATOM | 3314 | C   | LYS | 453 | 10.616 | -24.214 | 32.386 | 1.00 | 0.00 | 3A7 |
| ATOM | 3315 | O   | LYS | 453 | 9.869  | -23.577 | 33.112 | 1.00 | 0.00 | 3A7 |
| ATOM | 3316 | N   | LEU | 454 | 11.836 | -24.594 | 32.812 | 1.00 | 0.00 | 3A7 |
| ATOM | 3317 | CA  | LEU | 454 | 12.304 | -24.349 | 34.154 | 1.00 | 0.00 | 3A7 |
| ATOM | 3318 | CB  | LEU | 454 | 13.614 | -25.110 | 34.423 | 1.00 | 0.00 | 3A7 |
| ATOM | 3319 | CG  | LEU | 454 | 13.420 | -26.655 | 34.462 | 1.00 | 0.00 | 3A7 |
| ATOM | 3320 | CD1 | LEU | 454 | 14.712 | -27.380 | 34.874 | 1.00 | 0.00 | 3A7 |
| ATOM | 3321 | CD2 | LEU | 454 | 12.265 | -27.101 | 35.377 | 1.00 | 0.00 | 3A7 |
| ATOM | 3322 | C   | LEU | 454 | 12.488 | -22.881 | 34.440 | 1.00 | 0.00 | 3A7 |
| ATOM | 3323 | O   | LEU | 454 | 12.033 | -22.383 | 35.465 | 1.00 | 0.00 | 3A7 |
| ATOM | 3324 | N   | ALA | 455 | 13.101 | -22.129 | 33.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 3325 | CA  | ALA | 455 | 13.303 | -20.699 | 33.621 | 1.00 | 0.00 | 3A7 |
| ATOM | 3326 | CB  | ALA | 455 | 14.157 | -20.149 | 32.468 | 1.00 | 0.00 | 3A7 |
| ATOM | 3327 | C   | ALA | 455 | 12.006 | -19.916 | 33.668 | 1.00 | 0.00 | 3A7 |
| ATOM | 3328 | O   | ALA | 455 | 11.803 | -19.112 | 34.569 | 1.00 | 0.00 | 3A7 |
| ATOM | 3329 | N   | LEU | 456 | 11.065 | -20.169 | 32.730 | 1.00 | 0.00 | 3A7 |
| ATOM | 3330 | CA  | LEU | 456 | 9.795  | -19.468 | 32.642 | 1.00 | 0.00 | 3A7 |
| ATOM | 3331 | CB  | LEU | 456 | 9.033  | -19.835 | 31.351 | 1.00 | 0.00 | 3A7 |
| ATOM | 3332 | CG  | LEU | 456 | 9.514  | -19.139 | 30.053 | 1.00 | 0.00 | 3A7 |
| ATOM | 3333 | CD1 | LEU | 456 | 10.961 | -18.619 | 30.084 | 1.00 | 0.00 | 3A7 |
| ATOM | 3334 | CD2 | LEU | 456 | 9.277  | -20.054 | 28.836 | 1.00 | 0.00 | 3A7 |
| ATOM | 3335 | C   | LEU | 456 | 8.902  | -19.770 | 33.817 | 1.00 | 0.00 | 3A7 |
| ATOM | 3336 | O   | LEU | 456 | 8.226  | -18.888 | 34.337 | 1.00 | 0.00 | 3A7 |
| ATOM | 3337 | N   | VAL | 457 | 8.933  | -21.025 | 34.323 | 1.00 | 0.00 | 3A7 |
| ATOM | 3338 | CA  | VAL | 457 | 8.191  | -21.445 | 35.499 | 1.00 | 0.00 | 3A7 |
| ATOM | 3339 | CB  | VAL | 457 | 8.444  | -22.911 | 35.843 | 1.00 | 0.00 | 3A7 |
| ATOM | 3340 | CG1 | VAL | 457 | 8.005  | -23.325 | 37.263 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3341 | CG2 | VAL | 457 | 7.670  | -23.765 | 34.841 | 1.00 | 0.00 | 3A7 |
| ATOM | 3342 | C   | VAL | 457 | 8.576  | -20.633 | 36.694 | 1.00 | 0.00 | 3A7 |
| ATOM | 3343 | O   | VAL | 457 | 7.731  | -20.161 | 37.444 | 1.00 | 0.00 | 3A7 |
| ATOM | 3344 | N   | ARG | 458 | 9.892  | -20.443 | 36.892 | 1.00 | 0.00 | 3A7 |
| ATOM | 3345 | CA  | ARG | 458 | 10.419 | -19.722 | 38.015 | 1.00 | 0.00 | 3A7 |
| ATOM | 3346 | CB  | ARG | 458 | 11.926 | -19.996 | 38.164 | 1.00 | 0.00 | 3A7 |
| ATOM | 3347 | CG  | ARG | 458 | 12.246 | -21.369 | 38.758 | 1.00 | 0.00 | 3A7 |
| ATOM | 3348 | CD  | ARG | 458 | 13.750 | -21.581 | 38.977 | 1.00 | 0.00 | 3A7 |
| ATOM | 3349 | NE  | ARG | 458 | 14.409 | -21.751 | 37.641 | 1.00 | 0.00 | 3A7 |
| ATOM | 3350 | CZ  | ARG | 458 | 14.920 | -22.941 | 37.197 | 1.00 | 0.00 | 3A7 |
| ATOM | 3351 | NH1 | ARG | 458 | 15.570 | -22.979 | 35.995 | 1.00 | 0.00 | 3A7 |
| ATOM | 3352 | NH2 | ARG | 458 | 14.813 | -24.080 | 37.937 | 1.00 | 0.00 | 3A7 |
| ATOM | 3353 | C   | ARG | 458 | 10.219 | -18.233 | 37.894 | 1.00 | 0.00 | 3A7 |
| ATOM | 3354 | O   | ARG | 458 | 9.873  | -17.578 | 38.869 | 1.00 | 0.00 | 3A7 |
| ATOM | 3355 | N   | VAL | 459 | 10.398 | -17.640 | 36.691 | 1.00 | 0.00 | 3A7 |
| ATOM | 3356 | CA  | VAL | 459 | 10.219 | -16.217 | 36.448 | 1.00 | 0.00 | 3A7 |
| ATOM | 3357 | CB  | VAL | 459 | 10.629 | -15.894 | 35.017 | 1.00 | 0.00 | 3A7 |
| ATOM | 3358 | CG1 | VAL | 459 | 10.199 | -14.508 | 34.526 | 1.00 | 0.00 | 3A7 |
| ATOM | 3359 | CG2 | VAL | 459 | 12.165 | -16.014 | 34.950 | 1.00 | 0.00 | 3A7 |
| ATOM | 3360 | C   | VAL | 459 | 8.793  | -15.789 | 36.752 | 1.00 | 0.00 | 3A7 |
| ATOM | 3361 | O   | VAL | 459 | 8.553  | -14.855 | 37.511 | 1.00 | 0.00 | 3A7 |
| ATOM | 3362 | N   | LEU | 460 | 7.804  | -16.538 | 36.226 | 1.00 | 0.00 | 3A7 |
| ATOM | 3363 | CA  | LEU | 460 | 6.397  | -16.237 | 36.374 | 1.00 | 0.00 | 3A7 |
| ATOM | 3364 | CB  | LEU | 460 | 5.571  | -17.011 | 35.340 | 1.00 | 0.00 | 3A7 |
| ATOM | 3365 | CG  | LEU | 460 | 5.883  | -16.588 | 33.893 | 1.00 | 0.00 | 3A7 |
| ATOM | 3366 | CD1 | LEU | 460 | 5.285  | -17.596 | 32.898 | 1.00 | 0.00 | 3A7 |
| ATOM | 3367 | CD2 | LEU | 460 | 5.418  | -15.150 | 33.610 | 1.00 | 0.00 | 3A7 |
| ATOM | 3368 | C   | LEU | 460 | 5.857  | -16.582 | 37.736 | 1.00 | 0.00 | 3A7 |
| ATOM | 3369 | O   | LEU | 460 | 4.817  | -16.068 | 38.141 | 1.00 | 0.00 | 3A7 |
| ATOM | 3370 | N   | GLN | 461 | 6.570  | -17.449 | 38.498 | 1.00 | 0.00 | 3A7 |
| ATOM | 3371 | CA  | GLN | 461 | 6.249  | -17.756 | 39.877 | 1.00 | 0.00 | 3A7 |
| ATOM | 3372 | CB  | GLN | 461 | 6.961  | -19.025 | 40.414 | 1.00 | 0.00 | 3A7 |
| ATOM | 3373 | CG  | GLN | 461 | 6.204  | -19.729 | 41.554 | 1.00 | 0.00 | 3A7 |
| ATOM | 3374 | CD  | GLN | 461 | 6.924  | -21.033 | 41.909 | 1.00 | 0.00 | 3A7 |
| ATOM | 3375 | OE1 | GLN | 461 | 7.856  | -21.463 | 41.220 | 1.00 | 0.00 | 3A7 |
| ATOM | 3376 | NE2 | GLN | 461 | 6.464  | -21.670 | 43.029 | 1.00 | 0.00 | 3A7 |
| ATOM | 3377 | C   | GLN | 461 | 6.618  | -16.632 | 40.808 | 1.00 | 0.00 | 3A7 |
| ATOM | 3378 | O   | GLN | 461 | 5.945  | -16.385 | 41.809 | 1.00 | 0.00 | 3A7 |
| ATOM | 3379 | N   | ASN | 462 | 7.741  | -15.950 | 40.487 | 1.00 | 0.00 | 3A7 |
| ATOM | 3380 | CA  | ASN | 462 | 8.378  | -15.014 | 41.373 | 1.00 | 0.00 | 3A7 |
| ATOM | 3381 | CB  | ASN | 462 | 9.917  | -15.166 | 41.353 | 1.00 | 0.00 | 3A7 |
| ATOM | 3382 | CG  | ASN | 462 | 10.321 | -16.436 | 42.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 3383 | OD1 | ASN | 462 | 10.091 | -17.563 | 41.666 | 1.00 | 0.00 | 3A7 |
| ATOM | 3384 | ND2 | ASN | 462 | 10.944 | -16.227 | 43.317 | 1.00 | 0.00 | 3A7 |
| ATOM | 3385 | C   | ASN | 462 | 8.026  | -13.582 | 41.041 | 1.00 | 0.00 | 3A7 |
| ATOM | 3386 | O   | ASN | 462 | 8.214  | -12.710 | 41.888 | 1.00 | 0.00 | 3A7 |
| ATOM | 3387 | N   | PHE | 463 | 7.542  | -13.284 | 39.807 | 1.00 | 0.00 | 3A7 |
| ATOM | 3388 | CA  | PHE | 463 | 7.396  | -11.906 | 39.372 | 1.00 | 0.00 | 3A7 |
| ATOM | 3389 | CB  | PHE | 463 | 8.606  | -11.416 | 38.535 | 1.00 | 0.00 | 3A7 |
| ATOM | 3390 | CG  | PHE | 463 | 9.889  | -11.494 | 39.308 | 1.00 | 0.00 | 3A7 |
| ATOM | 3391 | CD1 | PHE | 463 | 10.834 | -12.474 | 38.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 3392 | CD2 | PHE | 463 | 10.162 | -10.594 | 40.340 | 1.00 | 0.00 | 3A7 |
| ATOM | 3393 | CE1 | PHE | 463 | 12.021 | -12.568 | 39.714 | 1.00 | 0.00 | 3A7 |
| ATOM | 3394 | CE2 | PHE | 463 | 11.352 | -10.684 | 41.057 | 1.00 | 0.00 | 3A7 |
| ATOM | 3395 | CZ  | PHE | 463 | 12.280 | -11.673 | 40.747 | 1.00 | 0.00 | 3A7 |
| ATOM | 3396 | C   | PHE | 463 | 6.160  | -11.715 | 38.530 | 1.00 | 0.00 | 3A7 |
| ATOM | 3397 | O   | PHE | 463 | 5.693  | -12.637 | 37.862 | 1.00 | 0.00 | 3A7 |
| ATOM | 3398 | N   | SER | 464 | 5.640  | -10.452 | 38.530 | 1.00 | 0.00 | 3A7 |
| ATOM | 3399 | CA  | SER | 464 | 4.607  | -9.957  | 37.639 | 1.00 | 0.00 | 3A7 |
| ATOM | 3400 | CB  | SER | 464 | 3.437  | -9.228  | 38.330 | 1.00 | 0.00 | 3A7 |
| ATOM | 3401 | OG  | SER | 464 | 3.854  | -8.156  | 39.167 | 1.00 | 0.00 | 3A7 |
| ATOM | 3402 | C   | SER | 464 | 5.295  | -9.043  | 36.654 | 1.00 | 0.00 | 3A7 |
| ATOM | 3403 | O   | SER | 464 | 5.987  | -8.102  | 37.035 | 1.00 | 0.00 | 3A7 |
| ATOM | 3404 | N   | PHE | 465 | 5.122  | -9.324  | 35.343 | 1.00 | 0.00 | 3A7 |
| ATOM | 3405 | CA  | PHE | 465 | 5.823  | -8.646  | 34.275 | 1.00 | 0.00 | 3A7 |
| ATOM | 3406 | CB  | PHE | 465 | 6.320  | -9.627  | 33.195 | 1.00 | 0.00 | 3A7 |
| ATOM | 3407 | CG  | PHE | 465 | 7.476  | -10.312 | 33.835 | 1.00 | 0.00 | 3A7 |
| ATOM | 3408 | CD1 | PHE | 465 | 7.317  | -11.547 | 34.451 | 1.00 | 0.00 | 3A7 |
| ATOM | 3409 | CD2 | PHE | 465 | 8.689  | -9.634  | 33.959 | 1.00 | 0.00 | 3A7 |
| ATOM | 3410 | CE1 | PHE | 465 | 8.353  | -12.080 | 35.204 | 1.00 | 0.00 | 3A7 |
| ATOM | 3411 | CE2 | PHE | 465 | 9.736  | -10.176 | 34.692 | 1.00 | 0.00 | 3A7 |
| ATOM | 3412 | CZ  | PHE | 465 | 9.564  | -11.399 | 35.322 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |        |        |      |      |     |
|------|------|-----|-----|-----|--------|--------|--------|------|------|-----|
| ATOM | 3413 | C   | PHE | 465 | 4.919  | -7.687 | 33.592 | 1.00 | 0.00 | 3A7 |
| ATOM | 3414 | O   | PHE | 465 | 3.724  | -7.936 | 33.425 | 1.00 | 0.00 | 3A7 |
| ATOM | 3415 | N   | LYS | 466 | 5.493  | -6.560 | 33.115 | 1.00 | 0.00 | 3A7 |
| ATOM | 3416 | CA  | LYS | 466 | 4.734  | -5.582 | 32.382 | 1.00 | 0.00 | 3A7 |
| ATOM | 3417 | CB  | LYS | 466 | 4.290  | -4.427 | 33.296 | 1.00 | 0.00 | 3A7 |
| ATOM | 3418 | CG  | LYS | 466 | 3.397  | -4.837 | 34.480 | 1.00 | 0.00 | 3A7 |
| ATOM | 3419 | CD  | LYS | 466 | 2.972  | -3.643 | 35.348 | 1.00 | 0.00 | 3A7 |
| ATOM | 3420 | CE  | LYS | 466 | 2.140  | -4.046 | 36.574 | 1.00 | 0.00 | 3A7 |
| ATOM | 3421 | NZ  | LYS | 466 | 2.919  | -4.922 | 37.481 | 1.00 | 0.00 | 3A7 |
| ATOM | 3422 | C   | LYS | 466 | 5.602  | -5.043 | 31.290 | 1.00 | 0.00 | 3A7 |
| ATOM | 3423 | O   | LYS | 466 | 6.771  | -4.756 | 31.526 | 1.00 | 0.00 | 3A7 |
| ATOM | 3424 | N   | PRO | 467 | 5.061  | -4.811 | 30.080 | 1.00 | 0.00 | 3A7 |
| ATOM | 3425 | CA  | PRO | 467 | 5.708  | -4.063 | 29.024 | 1.00 | 0.00 | 3A7 |
| ATOM | 3426 | CD  | PRO | 467 | 3.897  | -5.529 | 29.577 | 1.00 | 0.00 | 3A7 |
| ATOM | 3427 | CB  | PRO | 467 | 4.867  | -4.318 | 27.759 | 1.00 | 0.00 | 3A7 |
| ATOM | 3428 | CG  | PRO | 467 | 4.104  | -5.604 | 28.064 | 1.00 | 0.00 | 3A7 |
| ATOM | 3429 | C   | PRO | 467 | 5.709  | -2.585 | 29.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 3430 | O   | PRO | 467 | 4.657  | -2.040 | 29.696 | 1.00 | 0.00 | 3A7 |
| ATOM | 3431 | N   | CYS | 468 | 6.875  | -1.912 | 29.284 | 1.00 | 0.00 | 3A7 |
| ATOM | 3432 | CA  | CYS | 468 | 7.012  | -0.524 | 29.684 | 1.00 | 0.00 | 3A7 |
| ATOM | 3433 | CB  | CYS | 468 | 8.466  | -0.147 | 30.062 | 1.00 | 0.00 | 3A7 |
| ATOM | 3434 | SG  | CYS | 468 | 9.057  | -1.091 | 31.487 | 1.00 | 0.00 | 3A7 |
| ATOM | 3435 | C   | CYS | 468 | 6.616  | 0.383  | 28.544 | 1.00 | 0.00 | 3A7 |
| ATOM | 3436 | O   | CYS | 468 | 6.411  | 1.583  | 28.713 | 1.00 | 0.00 | 3A7 |
| ATOM | 3437 | N   | LYS | 469 | 6.540  | -0.205 | 27.334 | 1.00 | 0.00 | 3A7 |
| ATOM | 3438 | CA  | LYS | 469 | 6.355  | 0.499  | 26.104 | 1.00 | 0.00 | 3A7 |
| ATOM | 3439 | CB  | LYS | 469 | 7.640  | 0.501  | 25.281 | 1.00 | 0.00 | 3A7 |
| ATOM | 3440 | CG  | LYS | 469 | 8.757  | 1.350  | 25.918 | 1.00 | 0.00 | 3A7 |
| ATOM | 3441 | CD  | LYS | 469 | 10.000 | 1.530  | 25.028 | 1.00 | 0.00 | 3A7 |
| ATOM | 3442 | CE  | LYS | 469 | 9.788  | 2.435  | 23.807 | 1.00 | 0.00 | 3A7 |
| ATOM | 3443 | NZ  | LYS | 469 | 9.393  | 3.802  | 24.218 | 1.00 | 0.00 | 3A7 |
| ATOM | 3444 | C   | LYS | 469 | 5.347  | -0.291 | 25.354 | 1.00 | 0.00 | 3A7 |
| ATOM | 3445 | O   | LYS | 469 | 5.575  | -1.459 | 25.050 | 1.00 | 0.00 | 3A7 |
| ATOM | 3446 | N   | GLU | 470 | 4.138  | 0.226  | 25.134 | 1.00 | 0.00 | 3A7 |
| ATOM | 3447 | CA  | GLU | 470 | 3.141  | -0.604 | 24.504 | 1.00 | 0.00 | 3A7 |
| ATOM | 3448 | CB  | GLU | 470 | 1.701  | -0.299 | 24.997 | 1.00 | 0.00 | 3A7 |
| ATOM | 3449 | CG  | GLU | 470 | 1.488  | -0.619 | 26.491 | 1.00 | 0.00 | 3A7 |
| ATOM | 3450 | CD  | GLU | 470 | 1.553  | -2.121 | 26.773 | 1.00 | 0.00 | 3A7 |
| ATOM | 3451 | OE1 | GLU | 470 | 1.559  | -2.928 | 25.806 | 1.00 | 0.00 | 3A7 |
| ATOM | 3452 | OE2 | GLU | 470 | 1.584  | -2.480 | 27.981 | 1.00 | 0.00 | 3A7 |
| ATOM | 3453 | C   | GLU | 470 | 3.348  | -0.317 | 23.071 | 1.00 | 0.00 | 3A7 |
| ATOM | 3454 | O   | GLU | 470 | 4.315  | -0.740 | 22.429 | 1.00 | 0.00 | 3A7 |
| ATOM | 3455 | N   | THR | 471 | 2.368  | 0.501  | 22.575 | 1.00 | 0.00 | 3A7 |
| ATOM | 3456 | CA  | THR | 471 | 2.160  | 1.284  | 21.360 | 1.00 | 0.00 | 3A7 |
| ATOM | 3457 | CB  | THR | 471 | 2.447  | 2.764  | 21.659 | 1.00 | 0.00 | 3A7 |
| ATOM | 3458 | OG1 | THR | 471 | 1.929  | 3.641  | 20.661 | 1.00 | 0.00 | 3A7 |
| ATOM | 3459 | CG2 | THR | 471 | 3.946  | 3.049  | 21.904 | 1.00 | 0.00 | 3A7 |
| ATOM | 3460 | C   | THR | 471 | 2.841  | 0.808  | 20.088 | 1.00 | 0.00 | 3A7 |
| ATOM | 3461 | O   | THR | 471 | 3.308  | 1.608  | 19.278 | 1.00 | 0.00 | 3A7 |
| ATOM | 3462 | N   | GLN | 472 | 2.875  | -0.535 | 19.884 | 1.00 | 0.00 | 3A7 |
| ATOM | 3463 | CA  | GLN | 472 | 3.410  | -1.235 | 18.731 | 1.00 | 0.00 | 3A7 |
| ATOM | 3464 | CB  | GLN | 472 | 2.623  | -0.915 | 17.428 | 1.00 | 0.00 | 3A7 |
| ATOM | 3465 | CG  | GLN | 472 | 2.830  | -1.913 | 16.270 | 1.00 | 0.00 | 3A7 |
| ATOM | 3466 | CD  | GLN | 472 | 2.412  | -3.322 | 16.703 | 1.00 | 0.00 | 3A7 |
| ATOM | 3467 | OE1 | GLN | 472 | 3.252  | -4.222 | 16.818 | 1.00 | 0.00 | 3A7 |
| ATOM | 3468 | NE2 | GLN | 472 | 1.077  | -3.502 | 16.944 | 1.00 | 0.00 | 3A7 |
| ATOM | 3469 | C   | GLN | 472 | 4.893  | -0.974 | 18.547 | 1.00 | 0.00 | 3A7 |
| ATOM | 3470 | O   | GLN | 472 | 5.362  | -0.673 | 17.450 | 1.00 | 0.00 | 3A7 |
| ATOM | 3471 | N   | ILE | 473 | 5.672  | -1.090 | 19.658 | 1.00 | 0.00 | 3A7 |
| ATOM | 3472 | CA  | ILE | 473 | 7.130  | -0.993 | 19.613 | 1.00 | 0.00 | 3A7 |
| ATOM | 3473 | CB  | ILE | 473 | 7.790  | -0.303 | 20.808 | 1.00 | 0.00 | 3A7 |
| ATOM | 3474 | CG2 | ILE | 473 | 9.304  | -0.020 | 20.648 | 1.00 | 0.00 | 3A7 |
| ATOM | 3475 | CG1 | ILE | 473 | 7.030  | 1.009  | 21.146 | 1.00 | 0.00 | 3A7 |
| ATOM | 3476 | CD  | ILE | 473 | 7.180  | 2.124  | 20.104 | 1.00 | 0.00 | 3A7 |
| ATOM | 3477 | C   | ILE | 473 | 7.840  | -2.153 | 19.174 | 1.00 | 0.00 | 3A7 |
| ATOM | 3478 | O   | ILE | 473 | 8.886  | -1.850 | 18.619 | 1.00 | 0.00 | 3A7 |
| ATOM | 3479 | N   | PRO | 474 | 7.388  | -3.403 | 19.312 | 1.00 | 0.00 | 3A7 |
| ATOM | 3480 | CA  | PRO | 474 | 8.307  | -4.483 | 19.289 | 1.00 | 0.00 | 3A7 |
| ATOM | 3481 | CD  | PRO | 474 | 6.293  | -3.751 | 20.216 | 1.00 | 0.00 | 3A7 |
| ATOM | 3482 | CB  | PRO | 474 | 7.554  | -5.688 | 19.660 | 1.00 | 0.00 | 3A7 |
| ATOM | 3483 | CG  | PRO | 474 | 6.580  | -5.162 | 20.707 | 1.00 | 0.00 | 3A7 |
| ATOM | 3484 | C   | PRO | 474 | 9.042  | -4.735 | 18.043 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3485 | O   | PRO | 474 | 8.461  | -4.845  | 16.967 | 1.00 | 0.00 | 3A7 |
| ATOM | 3486 | N   | LEU | 475 | 10.363 | -4.780  | 18.250 | 1.00 | 0.00 | 3A7 |
| ATOM | 3487 | CA  | LEU | 475 | 11.281 | -4.868  | 17.212 | 1.00 | 0.00 | 3A7 |
| ATOM | 3488 | CB  | LEU | 475 | 12.494 | -3.929  | 17.438 | 1.00 | 0.00 | 3A7 |
| ATOM | 3489 | CG  | LEU | 475 | 12.127 | -2.431  | 17.558 | 1.00 | 0.00 | 3A7 |
| ATOM | 3490 | CD1 | LEU | 475 | 13.371 | -1.592  | 17.906 | 1.00 | 0.00 | 3A7 |
| ATOM | 3491 | CD2 | LEU | 475 | 11.432 | -1.891  | 16.293 | 1.00 | 0.00 | 3A7 |
| ATOM | 3492 | C   | LEU | 475 | 11.786 | -6.229  | 17.109 | 1.00 | 0.00 | 3A7 |
| ATOM | 3493 | O   | LEU | 475 | 12.315 | -6.781  | 18.064 | 1.00 | 0.00 | 3A7 |
| ATOM | 3494 | N   | LYS | 476 | 11.627 | -6.792  | 15.915 | 1.00 | 0.00 | 3A7 |
| ATOM | 3495 | CA  | LYS | 476 | 12.112 | -8.088  | 15.588 | 1.00 | 0.00 | 3A7 |
| ATOM | 3496 | CB  | LYS | 476 | 11.115 | -8.801  | 14.712 | 1.00 | 0.00 | 3A7 |
| ATOM | 3497 | CG  | LYS | 476 | 9.772  | -9.009  | 15.441 | 1.00 | 0.00 | 3A7 |
| ATOM | 3498 | CD  | LYS | 476 | 8.674  | -9.612  | 14.555 | 1.00 | 0.00 | 3A7 |
| ATOM | 3499 | CE  | LYS | 476 | 8.939  | -11.068 | 14.167 | 1.00 | 0.00 | 3A7 |
| ATOM | 3500 | NZ  | LYS | 476 | 7.894  | -11.545 | 13.235 | 1.00 | 0.00 | 3A7 |
| ATOM | 3501 | C   | LYS | 476 | 13.325 | -7.870  | 14.776 | 1.00 | 0.00 | 3A7 |
| ATOM | 3502 | O   | LYS | 476 | 13.337 | -7.042  | 13.874 | 1.00 | 0.00 | 3A7 |
| ATOM | 3503 | N   | LEU | 477 | 14.395 | -8.621  | 15.042 | 1.00 | 0.00 | 3A7 |
| ATOM | 3504 | CA  | LEU | 477 | 15.554 | -8.551  | 14.210 | 1.00 | 0.00 | 3A7 |
| ATOM | 3505 | CB  | LEU | 477 | 16.856 | -8.930  | 14.889 | 1.00 | 0.00 | 3A7 |
| ATOM | 3506 | CG  | LEU | 477 | 18.083 | -8.017  | 14.617 | 1.00 | 0.00 | 3A7 |
| ATOM | 3507 | CD1 | LEU | 477 | 19.159 | -8.239  | 15.698 | 1.00 | 0.00 | 3A7 |
| ATOM | 3508 | CD2 | LEU | 477 | 18.705 | -8.182  | 13.223 | 1.00 | 0.00 | 3A7 |
| ATOM | 3509 | C   | LEU | 477 | 15.422 | -9.412  | 13.099 | 1.00 | 0.00 | 3A7 |
| ATOM | 3510 | O   | LEU | 477 | 14.926 | -10.517 | 13.208 | 1.00 | 0.00 | 3A7 |
| ATOM | 3511 | N   | ARG | 478 | 15.810 | -8.885  | 11.967 | 1.00 | 0.00 | 3A7 |
| ATOM | 3512 | CA  | ARG | 478 | 15.460 | -9.604  | 10.853 | 1.00 | 0.00 | 3A7 |
| ATOM | 3513 | CB  | ARG | 478 | 14.781 | -8.647  | 9.829  | 1.00 | 0.00 | 3A7 |
| ATOM | 3514 | CG  | ARG | 478 | 13.512 | -7.955  | 10.358 | 1.00 | 0.00 | 3A7 |
| ATOM | 3515 | CD  | ARG | 478 | 12.226 | -8.561  | 9.784  | 1.00 | 0.00 | 3A7 |
| ATOM | 3516 | NE  | ARG | 478 | 12.180 | -10.004 | 10.198 | 1.00 | 0.00 | 3A7 |
| ATOM | 3517 | CZ  | ARG | 478 | 11.186 | -10.528 | 10.977 | 1.00 | 0.00 | 3A7 |
| ATOM | 3518 | NH1 | ARG | 478 | 11.256 | -11.836 | 11.366 | 1.00 | 0.00 | 3A7 |
| ATOM | 3519 | NH2 | ARG | 478 | 10.121 | -9.764  | 11.352 | 1.00 | 0.00 | 3A7 |
| ATOM | 3520 | C   | ARG | 478 | 16.502 | -10.335 | 10.080 | 1.00 | 0.00 | 3A7 |
| ATOM | 3521 | O   | ARG | 478 | 16.245 | -10.652 | 8.927  | 1.00 | 0.00 | 3A7 |
| ATOM | 3522 | N   | PHE | 479 | 17.697 | -10.610 | 10.632 | 1.00 | 0.00 | 3A7 |
| ATOM | 3523 | CA  | PHE | 479 | 18.858 | -10.706 | 9.806  | 1.00 | 0.00 | 3A7 |
| ATOM | 3524 | CB  | PHE | 479 | 20.076 | -10.235 | 10.539 | 1.00 | 0.00 | 3A7 |
| ATOM | 3525 | CG  | PHE | 479 | 21.147 | -9.680  | 9.633  | 1.00 | 0.00 | 3A7 |
| ATOM | 3526 | CD1 | PHE | 479 | 20.917 | -8.497  | 8.929  | 1.00 | 0.00 | 3A7 |
| ATOM | 3527 | CD2 | PHE | 479 | 22.379 | -10.322 | 9.495  | 1.00 | 0.00 | 3A7 |
| ATOM | 3528 | CE1 | PHE | 479 | 21.894 | -7.970  | 8.093  | 1.00 | 0.00 | 3A7 |
| ATOM | 3529 | CE2 | PHE | 479 | 23.356 | -9.799  | 8.652  | 1.00 | 0.00 | 3A7 |
| ATOM | 3530 | CZ  | PHE | 479 | 23.115 | -8.622  | 7.951  | 1.00 | 0.00 | 3A7 |
| ATOM | 3531 | C   | PHE | 479 | 19.185 | -12.054 | 9.251  | 1.00 | 0.00 | 3A7 |
| ATOM | 3532 | O   | PHE | 479 | 20.077 | -12.120 | 8.413  | 1.00 | 0.00 | 3A7 |
| ATOM | 3533 | N   | GLY | 480 | 18.507 | -13.153 | 9.632  | 1.00 | 0.00 | 3A7 |
| ATOM | 3534 | CA  | GLY | 480 | 18.751 | -14.416 | 8.969  | 1.00 | 0.00 | 3A7 |
| ATOM | 3535 | C   | GLY | 480 | 19.990 | -15.080 | 9.499  | 1.00 | 0.00 | 3A7 |
| ATOM | 3536 | O   | GLY | 480 | 21.012 | -14.455 | 9.781  | 1.00 | 0.00 | 3A7 |
| ATOM | 3537 | N   | GLY | 481 | 19.874 | -16.400 | 9.691  | 1.00 | 0.00 | 3A7 |
| ATOM | 3538 | CA  | GLY | 481 | 20.747 | -17.199 | 10.480 | 1.00 | 0.00 | 3A7 |
| ATOM | 3539 | C   | GLY | 481 | 19.999 | -17.404 | 11.756 | 1.00 | 0.00 | 3A7 |
| ATOM | 3540 | O   | GLY | 481 | 19.686 | -18.530 | 12.126 | 1.00 | 0.00 | 3A7 |
| ATOM | 3541 | N   | LEU | 482 | 19.687 | -16.297 | 12.465 | 1.00 | 0.00 | 3A7 |
| ATOM | 3542 | CA  | LEU | 482 | 19.157 | -16.393 | 13.801 | 1.00 | 0.00 | 3A7 |
| ATOM | 3543 | CB  | LEU | 482 | 20.314 | -16.416 | 14.840 | 1.00 | 0.00 | 3A7 |
| ATOM | 3544 | CG  | LEU | 482 | 20.009 | -17.132 | 16.175 | 1.00 | 0.00 | 3A7 |
| ATOM | 3545 | CD1 | LEU | 482 | 18.926 | -16.443 | 17.020 | 1.00 | 0.00 | 3A7 |
| ATOM | 3546 | CD2 | LEU | 482 | 19.738 | -18.634 | 15.963 | 1.00 | 0.00 | 3A7 |
| ATOM | 3547 | C   | LEU | 482 | 18.293 | -15.192 | 13.998 | 1.00 | 0.00 | 3A7 |
| ATOM | 3548 | O   | LEU | 482 | 18.787 | -14.069 | 13.996 | 1.00 | 0.00 | 3A7 |
| ATOM | 3549 | N   | LEU | 483 | 16.972 | -15.412 | 14.210 | 1.00 | 0.00 | 3A7 |
| ATOM | 3550 | CA  | LEU | 483 | 16.003 | -14.371 | 14.462 | 1.00 | 0.00 | 3A7 |
| ATOM | 3551 | CB  | LEU | 483 | 14.571 | -14.799 | 14.069 | 1.00 | 0.00 | 3A7 |
| ATOM | 3552 | CG  | LEU | 483 | 14.356 | -14.905 | 12.543 | 1.00 | 0.00 | 3A7 |
| ATOM | 3553 | CD1 | LEU | 483 | 12.892 | -15.253 | 12.231 | 1.00 | 0.00 | 3A7 |
| ATOM | 3554 | CD2 | LEU | 483 | 14.772 | -13.634 | 11.775 | 1.00 | 0.00 | 3A7 |
| ATOM | 3555 | C   | LEU | 483 | 15.995 | -14.055 | 15.923 | 1.00 | 0.00 | 3A7 |
| ATOM | 3556 | O   | LEU | 483 | 15.799 | -14.926 | 16.767 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3557 | N   | LEU | 484 | 16.246 | -12.778 | 16.236 | 1.00 | 0.00 | 3A7 |
| ATOM | 3558 | CA  | LEU | 484 | 16.374 | -12.310 | 17.588 | 1.00 | 0.00 | 3A7 |
| ATOM | 3559 | CB  | LEU | 484 | 17.753 | -11.620 | 17.812 | 1.00 | 0.00 | 3A7 |
| ATOM | 3560 | CG  | LEU | 484 | 18.984 | -12.548 | 17.710 | 1.00 | 0.00 | 3A7 |
| ATOM | 3561 | CD1 | LEU | 484 | 20.271 | -11.745 | 17.445 | 1.00 | 0.00 | 3A7 |
| ATOM | 3562 | CD2 | LEU | 484 | 19.140 | -13.413 | 18.970 | 1.00 | 0.00 | 3A7 |
| ATOM | 3563 | C   | LEU | 484 | 15.345 | -11.234 | 17.861 | 1.00 | 0.00 | 3A7 |
| ATOM | 3564 | O   | LEU | 484 | 14.779 | -10.598 | 16.981 | 1.00 | 0.00 | 3A7 |
| ATOM | 3565 | N   | THR | 485 | 15.149 | -10.896 | 19.142 | 1.00 | 0.00 | 3A7 |
| ATOM | 3566 | CA  | THR | 485 | 14.449 | -9.702  | 19.526 | 1.00 | 0.00 | 3A7 |
| ATOM | 3567 | CB  | THR | 485 | 13.528 | -9.902  | 20.697 | 1.00 | 0.00 | 3A7 |
| ATOM | 3568 | OG1 | THR | 485 | 12.643 | -10.981 | 20.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 3569 | CG2 | THR | 485 | 12.694 | -8.634  | 20.978 | 1.00 | 0.00 | 3A7 |
| ATOM | 3570 | C   | THR | 485 | 15.542 | -8.739  | 19.870 | 1.00 | 0.00 | 3A7 |
| ATOM | 3571 | O   | THR | 485 | 16.525 | -9.095  | 20.514 | 1.00 | 0.00 | 3A7 |
| ATOM | 3572 | N   | GLU | 486 | 15.407 | -7.491  | 19.395 | 1.00 | 0.00 | 3A7 |
| ATOM | 3573 | CA  | GLU | 486 | 16.478 | -6.537  | 19.402 | 1.00 | 0.00 | 3A7 |
| ATOM | 3574 | CB  | GLU | 486 | 16.229 | -5.476  | 18.329 | 1.00 | 0.00 | 3A7 |
| ATOM | 3575 | CG  | GLU | 486 | 16.097 | -6.056  | 16.918 | 1.00 | 0.00 | 3A7 |
| ATOM | 3576 | CD  | GLU | 486 | 16.045 | -4.920  | 15.900 | 1.00 | 0.00 | 3A7 |
| ATOM | 3577 | OE1 | GLU | 486 | 15.044 | -4.847  | 15.140 | 1.00 | 0.00 | 3A7 |
| ATOM | 3578 | OE2 | GLU | 486 | 17.014 | -4.115  | 15.863 | 1.00 | 0.00 | 3A7 |
| ATOM | 3579 | C   | GLU | 486 | 16.763 | -5.904  | 20.729 | 1.00 | 0.00 | 3A7 |
| ATOM | 3580 | O   | GLU | 486 | 17.821 | -6.121  | 21.297 | 1.00 | 0.00 | 3A7 |
| ATOM | 3581 | N   | LYS | 487 | 15.871 | -5.074  | 21.275 | 1.00 | 0.00 | 3A7 |
| ATOM | 3582 | CA  | LYS | 487 | 16.181 | -4.394  | 22.523 | 1.00 | 0.00 | 3A7 |
| ATOM | 3583 | CB  | LYS | 487 | 16.681 | -2.935  | 22.345 | 1.00 | 0.00 | 3A7 |
| ATOM | 3584 | CG  | LYS | 487 | 18.078 | -2.831  | 21.710 | 1.00 | 0.00 | 3A7 |
| ATOM | 3585 | CD  | LYS | 487 | 18.582 | -1.386  | 21.553 | 1.00 | 0.00 | 3A7 |
| ATOM | 3586 | CE  | LYS | 487 | 17.737 | -0.521  | 20.606 | 1.00 | 0.00 | 3A7 |
| ATOM | 3587 | NZ  | LYS | 487 | 17.683 | -1.111  | 19.249 | 1.00 | 0.00 | 3A7 |
| ATOM | 3588 | C   | LYS | 487 | 14.847 | -4.380  | 23.208 | 1.00 | 0.00 | 3A7 |
| ATOM | 3589 | O   | LYS | 487 | 14.110 | -3.436  | 22.965 | 1.00 | 0.00 | 3A7 |
| ATOM | 3590 | N   | PRO | 488 | 14.469 | -5.369  | 24.036 | 1.00 | 0.00 | 3A7 |
| ATOM | 3591 | CA  | PRO | 488 | 13.160 | -5.418  | 24.666 | 1.00 | 0.00 | 3A7 |
| ATOM | 3592 | CD  | PRO | 488 | 15.099 | -6.687  | 23.995 | 1.00 | 0.00 | 3A7 |
| ATOM | 3593 | CB  | PRO | 488 | 12.772 | -6.900  | 24.541 | 1.00 | 0.00 | 3A7 |
| ATOM | 3594 | CG  | PRO | 488 | 14.103 | -7.653  | 24.646 | 1.00 | 0.00 | 3A7 |
| ATOM | 3595 | C   | PRO | 488 | 13.285 | -4.931  | 26.063 | 1.00 | 0.00 | 3A7 |
| ATOM | 3596 | O   | PRO | 488 | 14.207 | -5.350  | 26.760 | 1.00 | 0.00 | 3A7 |
| ATOM | 3597 | N   | ILE | 489 | 12.369 | -4.042  | 26.506 | 1.00 | 0.00 | 3A7 |
| ATOM | 3598 | CA  | ILE | 489 | 12.431 | -3.564  | 27.858 | 1.00 | 0.00 | 3A7 |
| ATOM | 3599 | CB  | ILE | 489 | 12.824 | -2.096  | 28.021 | 1.00 | 0.00 | 3A7 |
| ATOM | 3600 | CG2 | ILE | 489 | 14.258 | -1.923  | 27.475 | 1.00 | 0.00 | 3A7 |
| ATOM | 3601 | CG1 | ILE | 489 | 11.831 | -1.092  | 27.392 | 1.00 | 0.00 | 3A7 |
| ATOM | 3602 | CD  | ILE | 489 | 12.182 | 0.356   | 27.747 | 1.00 | 0.00 | 3A7 |
| ATOM | 3603 | C   | ILE | 489 | 11.136 | -3.837  | 28.577 | 1.00 | 0.00 | 3A7 |
| ATOM | 3604 | O   | ILE | 489 | 10.052 | -3.733  | 28.009 | 1.00 | 0.00 | 3A7 |
| ATOM | 3605 | N   | VAL | 490 | 11.230 | -4.209  | 29.878 | 1.00 | 0.00 | 3A7 |
| ATOM | 3606 | CA  | VAL | 490 | 10.101 | -4.648  | 30.674 | 1.00 | 0.00 | 3A7 |
| ATOM | 3607 | CB  | VAL | 490 | 9.925  | -6.155  | 30.572 | 1.00 | 0.00 | 3A7 |
| ATOM | 3608 | CG1 | VAL | 490 | 9.245  | -6.911  | 31.734 | 1.00 | 0.00 | 3A7 |
| ATOM | 3609 | CG2 | VAL | 490 | 9.143  | -6.483  | 29.279 | 1.00 | 0.00 | 3A7 |
| ATOM | 3610 | C   | VAL | 490 | 10.398 | -4.303  | 32.085 | 1.00 | 0.00 | 3A7 |
| ATOM | 3611 | O   | VAL | 490 | 11.537 | -4.064  | 32.455 | 1.00 | 0.00 | 3A7 |
| ATOM | 3612 | N   | LEU | 491 | 9.344  | -4.289  | 32.927 | 1.00 | 0.00 | 3A7 |
| ATOM | 3613 | CA  | LEU | 491 | 9.438  | -4.005  | 34.328 | 1.00 | 0.00 | 3A7 |
| ATOM | 3614 | CB  | LEU | 491 | 8.379  | -2.956  | 34.702 | 1.00 | 0.00 | 3A7 |
| ATOM | 3615 | CG  | LEU | 491 | 8.991  | -1.575  | 35.041 | 1.00 | 0.00 | 3A7 |
| ATOM | 3616 | CD1 | LEU | 491 | 7.898  | -0.495  | 35.142 | 1.00 | 0.00 | 3A7 |
| ATOM | 3617 | CD2 | LEU | 491 | 9.848  | -1.615  | 36.322 | 1.00 | 0.00 | 3A7 |
| ATOM | 3618 | C   | LEU | 491 | 9.183  | -5.273  | 35.064 | 1.00 | 0.00 | 3A7 |
| ATOM | 3619 | O   | LEU | 491 | 8.303  | -6.043  | 34.680 | 1.00 | 0.00 | 3A7 |
| ATOM | 3620 | N   | LYS | 492 | 9.934  | -5.530  | 36.165 | 1.00 | 0.00 | 3A7 |
| ATOM | 3621 | CA  | LYS | 492 | 9.855  | -6.761  | 36.930 | 1.00 | 0.00 | 3A7 |
| ATOM | 3622 | CB  | LYS | 492 | 11.254 | -7.391  | 37.203 | 1.00 | 0.00 | 3A7 |
| ATOM | 3623 | CG  | LYS | 492 | 12.184 | -6.661  | 38.201 | 1.00 | 0.00 | 3A7 |
| ATOM | 3624 | CD  | LYS | 492 | 12.735 | -5.301  | 37.743 | 1.00 | 0.00 | 3A7 |
| ATOM | 3625 | CE  | LYS | 492 | 12.568 | -4.191  | 38.784 | 1.00 | 0.00 | 3A7 |
| ATOM | 3626 | NZ  | LYS | 492 | 11.143 | -3.831  | 38.925 | 1.00 | 0.00 | 3A7 |
| ATOM | 3627 | C   | LYS | 492 | 9.148  | -6.537  | 38.247 | 1.00 | 0.00 | 3A7 |
| ATOM | 3628 | O   | LYS | 492 | 9.344  | -7.295  | 39.196 | 1.00 | 0.00 | 3A7 |

|      |      |     |     |     |        |         |        |      |      |     |
|------|------|-----|-----|-----|--------|---------|--------|------|------|-----|
| ATOM | 3629 | N   | ALA | 493 | 8.315  | -5.466  | 38.338 | 1.00 | 0.00 | 3A7 |
| ATOM | 3630 | CA  | ALA | 493 | 7.783  | -4.923  | 39.576 | 1.00 | 0.00 | 3A7 |
| ATOM | 3631 | CB  | ALA | 493 | 7.164  | -3.529  | 39.347 | 1.00 | 0.00 | 3A7 |
| ATOM | 3632 | C   | ALA | 493 | 6.735  | -5.798  | 40.223 | 1.00 | 0.00 | 3A7 |
| ATOM | 3633 | O   | ALA | 493 | 5.607  | -5.896  | 39.745 | 1.00 | 0.00 | 3A7 |
| ATOM | 3634 | N   | GLU | 494 | 7.121  | -6.449  | 41.348 | 1.00 | 0.00 | 3A7 |
| ATOM | 3635 | CA  | GLU | 494 | 6.270  | -7.353  | 42.081 | 1.00 | 0.00 | 3A7 |
| ATOM | 3636 | CB  | GLU | 494 | 6.221  | -8.771  | 41.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 3637 | CG  | GLU | 494 | 5.073  | -9.691  | 41.921 | 1.00 | 0.00 | 3A7 |
| ATOM | 3638 | CD  | GLU | 494 | 5.351  | -10.327 | 43.282 | 1.00 | 0.00 | 3A7 |
| ATOM | 3639 | OE1 | GLU | 494 | 6.416  | -10.984 | 43.425 | 1.00 | 0.00 | 3A7 |
| ATOM | 3640 | OE2 | GLU | 494 | 4.495  | -10.171 | 44.193 | 1.00 | 0.00 | 3A7 |
| ATOM | 3641 | C   | GLU | 494 | 6.833  | -7.451  | 43.468 | 1.00 | 0.00 | 3A7 |
| ATOM | 3642 | O   | GLU | 494 | 6.097  | -7.692  | 44.424 | 1.00 | 0.00 | 3A7 |
| ATOM | 3643 | N   | SER | 495 | 8.180  | -7.291  | 43.592 | 1.00 | 0.00 | 3A7 |
| ATOM | 3644 | CA  | SER | 495 | 9.005  | -7.634  | 44.741 | 1.00 | 0.00 | 3A7 |
| ATOM | 3645 | CB  | SER | 495 | 10.488 | -7.267  | 44.500 | 1.00 | 0.00 | 3A7 |
| ATOM | 3646 | OG  | SER | 495 | 10.963 | -7.890  | 43.315 | 1.00 | 0.00 | 3A7 |
| ATOM | 3647 | C   | SER | 495 | 8.584  | -6.990  | 46.046 | 1.00 | 0.00 | 3A7 |
| ATOM | 3648 | O   | SER | 495 | 8.318  | -5.791  | 46.117 | 1.00 | 0.00 | 3A7 |
| ATOM | 3649 | N   | ARG | 496 | 8.506  | -7.831  | 47.102 | 1.00 | 0.00 | 3A7 |
| ATOM | 3650 | CA  | ARG | 496 | 8.050  | -7.468  | 48.419 | 1.00 | 0.00 | 3A7 |
| ATOM | 3651 | CB  | ARG | 496 | 6.781  | -8.270  | 48.810 | 1.00 | 0.00 | 3A7 |
| ATOM | 3652 | CG  | ARG | 496 | 6.173  | -7.918  | 50.178 | 1.00 | 0.00 | 3A7 |
| ATOM | 3653 | CD  | ARG | 496 | 4.896  | -8.715  | 50.471 | 1.00 | 0.00 | 3A7 |
| ATOM | 3654 | NE  | ARG | 496 | 4.413  | -8.345  | 51.841 | 1.00 | 0.00 | 3A7 |
| ATOM | 3655 | CZ  | ARG | 496 | 3.354  | -8.981  | 52.430 | 1.00 | 0.00 | 3A7 |
| ATOM | 3656 | NH1 | ARG | 496 | 2.955  | -8.609  | 53.681 | 1.00 | 0.00 | 3A7 |
| ATOM | 3657 | NH2 | ARG | 496 | 2.696  | -9.982  | 51.778 | 1.00 | 0.00 | 3A7 |
| ATOM | 3658 | C   | ARG | 496 | 9.179  | -7.785  | 49.356 | 1.00 | 0.00 | 3A7 |
| ATOM | 3659 | O   | ARG | 496 | 9.927  | -8.738  | 49.139 | 1.00 | 0.00 | 3A7 |
| ATOM | 3660 | N   | ASP | 497 | 9.312  | -6.984  | 50.445 | 1.00 | 0.00 | 3A7 |
| ATOM | 3661 | CA  | ASP | 497 | 10.298 | -7.171  | 51.489 | 1.00 | 0.00 | 3A7 |
| ATOM | 3662 | CB  | ASP | 497 | 10.821 | -5.830  | 52.089 | 1.00 | 0.00 | 3A7 |
| ATOM | 3663 | CG  | ASP | 497 | 9.707  | -4.881  | 52.551 | 1.00 | 0.00 | 3A7 |
| ATOM | 3664 | OD1 | ASP | 497 | 8.940  | -4.387  | 51.682 | 1.00 | 0.00 | 3A7 |
| ATOM | 3665 | OD2 | ASP | 497 | 9.625  | -4.629  | 53.783 | 1.00 | 0.00 | 3A7 |
| ATOM | 3666 | C   | ASP | 497 | 9.711  | -8.068  | 52.560 | 1.00 | 0.00 | 3A7 |
| ATOM | 3667 | O   | ASP | 497 | 8.985  | -7.622  | 53.447 | 1.00 | 0.00 | 3A7 |
| ATOM | 3668 | N   | GLU | 498 | 10.021 | -9.384  | 52.458 | 1.00 | 0.00 | 3A7 |
| ATOM | 3669 | CA  | GLU | 498 | 9.495  | -10.423 | 53.314 | 1.00 | 0.00 | 3A7 |
| ATOM | 3670 | CB  | GLU | 498 | 8.919  | -11.610 | 52.501 | 1.00 | 0.00 | 3A7 |
| ATOM | 3671 | CG  | GLU | 498 | 7.782  | -11.185 | 51.557 | 1.00 | 0.00 | 3A7 |
| ATOM | 3672 | CD  | GLU | 498 | 7.253  | -12.413 | 50.822 | 1.00 | 0.00 | 3A7 |
| ATOM | 3673 | OE1 | GLU | 498 | 6.045  | -12.728 | 50.989 | 1.00 | 0.00 | 3A7 |
| ATOM | 3674 | OE2 | GLU | 498 | 8.050  | -13.049 | 50.081 | 1.00 | 0.00 | 3A7 |
| ATOM | 3675 | C   | GLU | 498 | 10.610 | -10.918 | 54.195 | 1.00 | 0.00 | 3A7 |
| ATOM | 3676 | O   | GLU | 498 | 11.726 | -10.403 | 54.157 | 1.00 | 0.00 | 3A7 |
| ATOM | 3677 | N   | THR | 499 | 10.311 | -11.961 | 55.010 | 1.00 | 0.00 | 3A7 |
| ATOM | 3678 | CA  | THR | 499 | 11.248 | -12.606 | 55.905 | 1.00 | 0.00 | 3A7 |
| ATOM | 3679 | CB  | THR | 499 | 10.615 | -12.970 | 57.245 | 1.00 | 0.00 | 3A7 |
| ATOM | 3680 | OG1 | THR | 499 | 9.418  | -13.726 | 57.084 | 1.00 | 0.00 | 3A7 |
| ATOM | 3681 | CG2 | THR | 499 | 10.291 | -11.664 | 57.998 | 1.00 | 0.00 | 3A7 |
| ATOM | 3682 | C   | THR | 499 | 11.798 | -13.836 | 55.217 | 1.00 | 0.00 | 3A7 |
| ATOM | 3683 | O   | THR | 499 | 11.311 | -14.244 | 54.163 | 1.00 | 0.00 | 3A7 |
| ATOM | 3684 | N   | VAL | 500 | 12.842 | -14.455 | 55.826 | 1.00 | 0.00 | 3A7 |
| ATOM | 3685 | CA  | VAL | 500 | 13.521 | -15.621 | 55.300 | 1.00 | 0.00 | 3A7 |
| ATOM | 3686 | CB  | VAL | 500 | 15.021 | -15.588 | 55.594 | 1.00 | 0.00 | 3A7 |
| ATOM | 3687 | CG1 | VAL | 500 | 15.312 | -15.508 | 57.109 | 1.00 | 0.00 | 3A7 |
| ATOM | 3688 | CG2 | VAL | 500 | 15.739 | -16.768 | 54.903 | 1.00 | 0.00 | 3A7 |
| ATOM | 3689 | C   | VAL | 500 | 12.857 | -16.864 | 55.847 | 1.00 | 0.00 | 3A7 |
| ATOM | 3690 | O   | VAL | 500 | 12.610 | -16.984 | 57.047 | 1.00 | 0.00 | 3A7 |
| ATOM | 3691 | N   | SER | 501 | 12.542 | -17.816 | 54.939 | 1.00 | 0.00 | 3A7 |
| ATOM | 3692 | CA  | SER | 501 | 11.904 | -19.059 | 55.286 | 1.00 | 0.00 | 3A7 |
| ATOM | 3693 | CB  | SER | 501 | 10.354 | -18.950 | 55.320 | 1.00 | 0.00 | 3A7 |
| ATOM | 3694 | OG  | SER | 501 | 9.744  | -20.142 | 55.806 | 1.00 | 0.00 | 3A7 |
| ATOM | 3695 | C   | SER | 501 | 12.356 | -20.035 | 54.235 | 1.00 | 0.00 | 3A7 |
| ATOM | 3696 | O   | SER | 501 | 12.898 | -21.094 | 54.550 | 1.00 | 0.00 | 3A7 |
| ATOM | 3697 | N   | GLY | 502 | 12.135 | -19.677 | 52.947 | 1.00 | 0.00 | 3A7 |
| ATOM | 3698 | CA  | GLY | 502 | 12.533 | -20.464 | 51.805 | 1.00 | 0.00 | 3A7 |
| ATOM | 3699 | C   | GLY | 502 | 13.587 | -19.693 | 51.074 | 1.00 | 0.00 | 3A7 |
| ATOM | 3700 | O   | GLY | 502 | 13.335 | -18.585 | 50.602 | 1.00 | 0.00 | 3A7 |



|        |      |       |     |     |        |         |        |      |      |     |
|--------|------|-------|-----|-----|--------|---------|--------|------|------|-----|
| ATOM   | 3701 | N     | ALA | 503 | 14.804 | -20.283 | 50.980 | 1.00 | 0.00 | 3A7 |
| ATOM   | 3702 | CA    | ALA | 503 | 15.970 | -19.715 | 50.338 | 1.00 | 0.00 | 3A7 |
| ATOM   | 3703 | CB    | ALA | 503 | 15.775 | -19.401 | 48.838 | 1.00 | 0.00 | 3A7 |
| ATOM   | 3704 | C     | ALA | 503 | 16.423 | -18.443 | 51.073 | 1.00 | 0.00 | 3A7 |
| ATOM   | 3705 | OT1   | ALA | 503 | 17.016 | -18.589 | 52.175 | 1.00 | 0.00 | 3A7 |
| ATOM   | 3706 | OT2   | ALA | 503 | 16.167 | -17.323 | 50.557 | 1.00 | 0.00 | 3A7 |
| TER    | 3707 |       | ALA | 503 |        |         |        |      |      |     |
| HETATM | 3708 | FE    | HEM | 600 | 19.802 | -26.909 | 18.195 | 1.00 | 0.00 | HEM |
| HETATM | 3709 | NA    | HEM | 600 | 19.117 | -26.973 | 16.343 | 1.00 | 0.00 | HEM |
| HETATM | 3710 | NB    | HEM | 600 | 18.291 | -25.763 | 18.746 | 1.00 | 0.00 | HEM |
| HETATM | 3711 | NC    | HEM | 600 | 20.542 | -26.830 | 20.017 | 1.00 | 0.00 | HEM |
| HETATM | 3712 | ND    | HEM | 600 | 21.332 | -28.034 | 17.616 | 1.00 | 0.00 | HEM |
| HETATM | 3713 | C1A   | HEM | 600 | 19.627 | -27.653 | 15.248 | 1.00 | 0.00 | HEM |
| HETATM | 3714 | C2A   | HEM | 600 | 18.787 | -27.461 | 14.072 | 1.00 | 0.00 | HEM |
| HETATM | 3715 | C3A   | HEM | 600 | 17.812 | -26.605 | 14.439 | 1.00 | 0.00 | HEM |
| HETATM | 3716 | C4A   | HEM | 600 | 17.993 | -26.338 | 15.849 | 1.00 | 0.00 | HEM |
| HETATM | 3717 | C1B   | HEM | 600 | 17.258 | -25.288 | 17.964 | 1.00 | 0.00 | HEM |
| HETATM | 3718 | C2B   | HEM | 600 | 16.334 | -24.465 | 18.724 | 1.00 | 0.00 | HEM |
| HETATM | 3719 | C3B   | HEM | 600 | 16.805 | -24.471 | 20.029 | 1.00 | 0.00 | HEM |
| HETATM | 3720 | C4B   | HEM | 600 | 18.026 | -25.267 | 20.000 | 1.00 | 0.00 | HEM |
| HETATM | 3721 | C1C   | HEM | 600 | 20.002 | -26.220 | 21.122 | 1.00 | 0.00 | HEM |
| HETATM | 3722 | C2C   | HEM | 600 | 20.837 | -26.398 | 22.303 | 1.00 | 0.00 | HEM |
| HETATM | 3723 | C3C   | HEM | 600 | 21.948 | -27.105 | 21.896 | 1.00 | 0.00 | HEM |
| HETATM | 3724 | C4C   | HEM | 600 | 21.734 | -27.359 | 20.473 | 1.00 | 0.00 | HEM |
| HETATM | 3725 | C1D   | HEM | 600 | 22.427 | -28.419 | 18.358 | 1.00 | 0.00 | HEM |
| HETATM | 3726 | C2D   | HEM | 600 | 23.355 | -29.229 | 17.581 | 1.00 | 0.00 | HEM |
| HETATM | 3727 | C3D   | HEM | 600 | 22.815 | -29.362 | 16.350 | 1.00 | 0.00 | HEM |
| HETATM | 3728 | C4D   | HEM | 600 | 21.589 | -28.591 | 16.366 | 1.00 | 0.00 | HEM |
| HETATM | 3729 | CHA   | HEM | 600 | 20.801 | -28.392 | 15.257 | 1.00 | 0.00 | HEM |
| HETATM | 3730 | CHB   | HEM | 600 | 17.121 | -25.582 | 16.615 | 1.00 | 0.00 | HEM |
| HETATM | 3731 | CHC   | HEM | 600 | 18.841 | -25.488 | 21.097 | 1.00 | 0.00 | HEM |
| HETATM | 3732 | CHD   | HEM | 600 | 22.615 | -28.078 | 19.676 | 1.00 | 0.00 | HEM |
| HETATM | 3733 | CMA   | HEM | 600 | 16.761 | -26.027 | 13.539 | 1.00 | 0.00 | HEM |
| HETATM | 3734 | CAA   | HEM | 600 | 18.874 | -28.152 | 12.738 | 1.00 | 0.00 | HEM |
| HETATM | 3735 | CBA   | HEM | 600 | 19.655 | -27.341 | 11.731 | 1.00 | 0.00 | HEM |
| HETATM | 3736 | CGA   | HEM | 600 | 19.868 | -28.082 | 10.424 | 1.00 | 0.00 | HEM |
| HETATM | 3737 | O1A   | HEM | 600 | 18.997 | -28.897 | 10.031 | 1.00 | 0.00 | HEM |
| HETATM | 3738 | O2A   | HEM | 600 | 20.918 | -27.812 | 9.777  | 1.00 | 0.00 | HEM |
| HETATM | 3739 | CMB   | HEM | 600 | 15.130 | -23.749 | 18.107 | 1.00 | 0.00 | HEM |
| HETATM | 3740 | CAB   | HEM | 600 | 16.311 | -23.874 | 21.208 | 1.00 | 0.00 | HEM |
| HETATM | 3741 | CBB   | HEM | 600 | 15.206 | -23.138 | 21.387 | 1.00 | 0.00 | HEM |
| HETATM | 3742 | CMC</ |     |     |        |         |        |      |      |     |

**Sequences :**

SEQ ID N°1: P450 Nor, crystal structure 1rom

SEQ ID N°2: P450 Ery F, crystal structure 1oxa

SEQ ID N°3: P450 Terp, crystal structure 1cpt

5 SEQ ID N°4: P450 Cam, crystal structure 3cpp

SEQ ID N°5: P450 BM3, crystal structure 2hpd

The sequence corresponding to the PDB structure includes 471 residues. For more clarity in Figure 1, the last 12 residues have been omitted, the C-terminal part having no equivalent counterpart in the other structures aligned.

10 SEQ ID N°6: P450 2C5, crystal structure 1dt6

Cyp2C5 from *Oryctolagus cuniculus* (Rabbit), with membrane spanning residues 3-21 deleted and a 4 residue histidine tag at the C-Terminus containing additional internal mutations.

SEQ ID N°7: P450 2C5 rabbit

15 Sequence corresponding to the non-mutated CYP 2C5 gene from *Oryctolagus cuniculus* (Rabbit), consistently with SwissProt CPC5\_RABIT P00179.

SEQ ID N° 8: CYP51, crystal structure 1e9x

Cyp51 from *Mycobacterium tuberculosis*, with a 4 residue histidine tag at the C-Terminus.

20 SEQ ID N°9: CYP3A1 rat

SEQ ID N°10: CYP3A3 human

Cytochrome P-450, a possible variant of CYP3A4, inducible by glucocorticoids in human liver.

SEQ ID N°11: CYP3A4 human

25 Numbering starts at Ala 1 (first residue Met is not included, consistently with SwissProt CP34\_HUMAN P08684)

SEQ ID N°12: CYP3A5 human

SEQ ID N°13: CYP3A43 human

SEQ ID N°14: CYP3A6 rabbit

30 SEQ ID N°15: CYP3A7 human

SEQ ID N°16: CYP3A12 dog

SEQ ID N°17: CYP3A29 pig

SEQ ID N°18: CYP3A13 mouse

**Figure 1: Structure-based alignment of human cytochromes P450 3A3, 3A4, 3A5, 3A7 and 3A43 and of selected mammalian P450 3A isozymes, with bacterial P450 crystal template structures and rabbit P450 2C5 crystal template structure.**

5 Sequence numbering is indicated for each enzyme of the structural template and for the human 3A4 and 3A7 isozymes, as examples given in the present invention. This alignment is first based on the structural alignment of bacterial P450s and rabbit P450 2C5 derived from GOK analysis. Human P450 3A sequences were then aligned with in-house tools that locates the CSBs on the target sequence. The  
10 alignment shown outside the CSBs is not relevant, as there is no structural information available in these regions. The CSB sequences are indicated by bold uppercase characters and are highlighted in grey. Amino acids strictly conserved between CYP3A and 2C5, or between CYP3A and all the sequences of crystal structures, are highlighted in black.

15 **Figure 2: Ramachandran plot of a lowest energy model of CYP3A4 produced by DYANA-XPLOR calculations from the six-template structural alignment.**

**Figure 3: view of one optimized CYP3A4 model. This figure can be replaced by the whole set of coordinates file of table 3 in the PDB format.**

**Figure 4: final position of testosterone into the CYP3A4 and CYP3A7 active sites after soft-restrained dynamics docking. The active sites are characterized by six Substrates Recognition Sites (SRS, after Gotoh 1989, in bold) associated to fragments of secondary element structures (in italic).**  
20

**Panel 4A In CYP3A4 active site, the docked testosterone molecule is oriented so that the A steroid cycle (carrying in position 3 a carbonyl function with an oxygen atom symbolized by a large ball ) is close to the hemic iron. This supports the propensity of CYP3A4 to metabolize testosterone in 6  $\beta$  position as indicated by the black solid arrow.**  
25

**Panel 4B In CYP3A7 active site, the docked testosterone molecule is oriented so that the D steroid cycle (carrying in position 17 a hydroxylic function with an oxygen atom symbolized by a large ball ) is close to the hemic iron. This supports the propensity of CYP3A7 to metabolize testosterone in 16  $\alpha$  position as indicated by the black solid arrow**  
30

**Figure 5: Energy profile of the soft-restrained dynamics docking of testosterone into CYP3A4 model.**

**Example 1: Determination of the 3D-structure of P450 3A4.**

5 ***Material***

The coordinates of the six P450 crystal structures: P450cam (3cpp), P450terp (1cpt), P450BM-3 (2hpd), P450eryF (1oxa), P450 nor (1rom) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank. The structural alignment and the conserved regions determination were realized using the GOK software  
10 (Jean et al. 1997) running on an Octane Silicon-Graphics workstation. Structures were built using the DYANA (Güntert et al. 1997), and X-PLOR softwares (Brünger 1992). Docking studies were performed with SYBYL 6.6 (Tripos Inc.) and TRIPOS force field. The structures were analyzed using Procheck-NMR (Laskowski et al. 1993) and visualized under SYBYL 6.6 (Tripos Inc.).

15

***Common Structural Blocks (CSB) determination.***

The first key point of this homology modeling study is the identification of the structural elements (hereafter designed as CSBs for Common Structural Blocks) conserved among the family of cytochromes P450 of known 3D structures, and the  
20 localization of these elements in the target sequence. These two tasks are performed using the GOK software (Jean et al. 1997), and are well described in a forthcoming article (Minoletti et al., *Proteins, Structure, Function and Genetics*, 2002). In brief, the basic idea of CSB identification by GOK is to use an internal coordinate representation –  $(\alpha, \tau)$  in our case (another representation of  $\phi$ ,  $\psi$  and  $\omega$  angles) –  
25 and to search for fragments in the six-template proteins having similar local trajectories in the internal coordinate space. GOK provides two adjustable parameters (the  $\alpha$ -mesh and the  $\alpha$ -margin) that define the tolerance on the comparison of the trajectories. These parameters were adjusted recursively to values ranging from 15 to 30° ( $\alpha$ -mesh) and 1 to 3 ( $\alpha$ -margin in mesh units). The  
30 evaluation of the quality of the match was measured using two multiple-way rmsd calculated in the cartesian coordinates space: mp-rms (the mean of all pairwise rms deviations) and s-rms (the mean of the deviations calculated with respect to a mean structure obtained from the average internal coordinates). For the different CSBs,

mp-rms value ranged between 0.3 and 4.9 Å in average, and s-rms between 0.04 and 2.4 Å.

***CYP3A4 sequence alignment and evaluation of the profile***

5 The multiple sequence alignment derived from the CSB identification was then used to build a similarity profile. The profile is defined as a position-specific scoring table created from aligned gap-free segments such as CSBs (Jean et al. 1997). The alignment then consists in a search of the best match (as per the best score) between a CSB of sequences defined structurally (*i.e.* independently of the  
10 nature of the aligned residues) and several other sequences that are well-aligned and exhibit a high sequence identity. In the P450 3A subfamily, many proteins exhibit high sequence identity. We extended our profile search program to take this information into account, *i.e.* to align the profile with a pre-defined multiple alignment of the cytochromes P450 3A subfamily members sequences (Gotoh 1992;  
15 Nelson et al. 1996). The similarity score was calculated using BLOSUM62 matrix (Henikoff and Henikoff 1992). The in-house tool SmartConsAlign (Atelier de Bio-informatique, Université Paris VI) described in Jean et al. 1997, allows to move the consensus matrix along the multiple sequence alignment of P450 3A family, and computes for each position a score of similarity. The best alignment found of  
20 CYP3A4 on CSBs is shown in Figure 1.

Once the alignment is completed, the 3D model rebuilding process can incorporate the atom Cartesian coordinates of the template structures only for amino acids located in structurally conserved regions (*i.e.* the CSBs). The coordinates of any of the template structures can be used for determining the final template. In each CSB,  
25 amino acid positions have been renumbered according to the sequence of human P450 3A4. At a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the modeled (target) residue. When residues differ, only the coordinates of the backbone atoms are assigned ( $C\alpha$ ), and sometimes  $C\beta$  when they  
30 exist. Side chains are rebuilt from libraries giving the most probable rotamers for each amino acid (see below). In some cases, it was possible to superimpose the positions of carbon atoms of lateral chains up to ranks  $\gamma$  and  $\delta$  along the sidechain, thus explicitly defining a unique rotamer.

For amino acids located outside the CSBs (structurally variable zones that include generally loops), the rebuilding is more complex, and can be done only after rebuilding of structurally conserved zones. In the multiple structural alignment (Figure 1), the regions separating the CSBs bring no structural information at all.

- 5 Short loops are rebuilt entirely, since solutions of acceptable geometry for atoms are in limited number, *i.e.* the lowest energy drives the selection of the good geometry. For longer segments, various structures are provided by the constrained minimization runs, and a manual selection is operated.

#### 10 *Constraints derivation and rebuilding*

- A strategy inspired of the techniques commonly used to built structures from NMR data (Patard et al. 1996) is applied. The main idea is to express all available information issued from the comparison of the templates in term of geometrical constraints (distances and angles). Each constraint will be defined as an interval (for
- 15 a given pair of atoms, this is the average of the six atom-atom distances found in the template structures +/- the standard deviation), similarly to the strategy developed by Havel and Snow (Havel and Snow 1991). However, the number of constraints corresponding to all atom-atom distances, for example, would be prohibitive for a protein of the size of the P450 (around 1,000,000 inter-residual distances if we
- 20 consider 250 conserved residues and an average of four atoms per residues). Previous NMR studies (Patard et al. 1996) have shown that local constraints are sufficient to allow a correct reconstruction of a structure. This reduces drastically the number of constraints needed, and increases the flexibility of the model. In addition, similarly to what is done in protein structure determination by NMR, we
- 25 can build a family of structures instead of a single model. This allows an easier analysis of the well or less well-predicted regions. This is also an advantage for the analysis of the side-chain positions, particularly in prevision of a substrate docking study. Finally, the loops are passively reconstructed with the rest of the structure. The only specific information we have introduced in variable regions was to guide
- 30 all their residues to an allowed region of the Ramachandran diagram. Indeed, analysis of well-defined structures shows that nearly all residues, including those of the loops, should belong to an allowed region. The lower the proportion of residues

found outside the allowed Ramachandran regions, the better the structure is. This criterion of quality has been applied to derive the model described herein.

Accordingly, we retained for model rebuilding all the distance and angle intervals corresponding to the following principles:

- 5 - all distances for which the lower boundary was less than 8 Å. This cutoff is totally sufficient to ensure, at least, the formation of the local structure elements. Such a cutoff is relatively high and thus costly in terms of size of constraints file, but proved necessary to ensure good results for the P450s. This may be due to the fact that P450 enzymes are mostly formed of  $\alpha$ -helices, the average distance between  
10 two helices being larger than between two adjacent  $\beta$ -strands. In addition, the percentage of residues located outside CSBs is rather high in the structural alignment of P450s, and a better convergence can be obtained only at the expense of a high number of rebuilding distance constraints.
- all the distances involving at least one side-chain atom, to preserve the spatial  
15 arrangement between CSBs
- finally, all the distances involving atoms of the heme group, to fix as much as possible the neighborhood of the iron atom.

The total number of distance constraints was, in these conditions, equal to 58506.

- Similarly, angular constraints were calculated in each building block. A CSB is  
20 indeed defined as a conserved trajectory in the  $\phi, \psi$  coordinates space (or  $\alpha, \tau$ ). Thus, dihedral angles  $\phi$  and  $\psi$  of all residues located in CSBs can be defined as constraints, given by the average values of corresponding  $\phi, \psi$  angles in the six templates +/- the standard deviation. To these backbone dihedral angles, can be added the side chains torsion angles  $\chi_1, \chi_2$  whenever possible, as determined by the  
25 rotamer selection. The total number of dihedral angle constraints was, in these conditions, equal to 761.

### ***Rotamer selection***

- In proteins, the preferential orientation of the side chain ( $60^\circ, -60^\circ, 180^\circ$ ) depends  
30 on the local conformation of the residue, and thus on the nature of the secondary structure in which the residue is involved. According to the rotamer library built by Karplus and coll. (Dunbrack and Karplus 1993), to a given  $(\phi, \psi)$  couple in the

Ramachandran diagram can be associated a specific rotamer for each type of residue. These tables have been used to determine the most probable rotamer for each residue located in CSB, except when there are conserved atoms in the side chain that assign unambiguously a rotamer ( $\chi_1$ ,  $\chi_2$ ). The selected ( $\chi_1$ ,  $\chi_2$ ) couples  
5 were included in the above-mentioned set of angle 761 dihedral constraints.

### ***Structure calculation and optimization***

We used a procedure similar to structure calculation starting from NMR constraints. A first set of structures was calculated using the DYANA software (Güntert et al.  
10 1997) and the 58506 distance and 761 angular constraints. Families of structures are generated. The energy of each structure is minimized with the procedure vtfmin in DYANA.

Due to the size and the amount of loops in the molecule, some structures presented topological defects and were discarded. The others were further optimized by using  
15 the X-PLOR software. A set of constraints was added at this stage in order to guide the loop residues to the nearest allowed region in the Ramachandran diagram. The topology and parameter files of CHARMM22 were used. The electrostatic term was turned off.

The DYANA software is unable to deal with disconnected objects. A new residue  
20 type was, thus, added to the standard amino acid library to take into account the the presence of the heme. This residue was obtained by combining the heme to a cysteine and was inserted at position 441 in the sequence of the protein (**Figure 1**).

### **Description of the CYP3A4 Model**

25 We rebuilt a model of the protein depleted of its first 50 residues (N-terminal domain). This segment is highly hydrophobic, and supposed to form the anchor of the protein in the membrane. There is no structural information about this putative transmembrane domain, and this segment was thus not incorporated into the modeling process, and in the final model. Such a "free" segment (with no  
30 constraints) would perturbate the convergence of computation or the stability of the whole rebuilt structure.

The quality of the various structures optimized under XPLOR was checked for the stereochemical quality (backbone and side chain conformation) by PROCHECK



(Laskowski et al. 1993). The Ramachandran plot shows that our six-template approach generated converging models, possessing the same fold. The lowest energy models had 73% of their non-glycine and non-proline residues with  $\phi$ ,  $\psi$  conformation in the most favoured regions of the Ramachandran plot (core region),  
5 20% in additional allowed regions, and 5% in the generously allowed regions. Only 2.3% (9 residues) had their  $\phi$ ,  $\psi$  conformation in disallowed regions (**Figure 2**). The total number of residues in the model is 452; which 399 are non-glycine and non-proline residues, and number of residues in the native sequence is 502.

When compared to the CYP2C5 crystal structure, it can be noticed that the  
10 CYP3A4 model exhibits a good 3D similarity in the global fold than expected, since this structure counts only for one in the six-template approach. This proves that in this approach, there is no “averaging” effect, *i.e.* the mammalian structure had a decisive influence over the five bacterial (and fungus) templates. Our final fold of CYP3A4 is very consistent with a mammalian one, despite the fact that it has been  
15 rebuilt by using the structural information contained in non-mammalian cytochromes P450.

The active site is delimited by the six substrate recognition sites (SRS) that have been first identified and described by Gotoh (Gotoh 1992) from the unique structure available in the early 1990s (P450<sub>cam</sub>), and that are today commonly accepted for  
20 depicting substrate recognition by various cytochromes P450 (especially from the family 2, but extended to other P450 families). These sites are associated with the active site and are located in the less conserved regions of the CYPs, thus possibly accounting for the various substrate specificity among P450s. When comparing our various optimized structures, it is found that SRS1 (100-125, includes helix B), SRS  
25 2 (205-218, includes C-terminus of helix F), and SRS3 (237-249, includes N-terminus part of helix G) are located in less-defined regions, with significant variability in spatial position (flexibility). These regions correspond also to parts of the sequence that are less well-aligned. At the opposite, the SRS4 (295-320, central part of helix I), SRS5 (363-380, C-term of helix K and  $\beta$ -sheet  $\beta$ 1-4) and SRS6  
30 (470-490,  $\beta$ -sheets  $\beta$ 4-1 and  $\beta$ 4-2) are well-defined fragments of the structures. SRS4 and SRS5 segments in particular are correlated to regions in the sequence that are unequivocally aligned.

The only model structure of CYP3A4 that has been described in the literature and that we can handle for structural comparison, is that of Szklarz and Halpert, derived from a multiple-template approach (four-bacterial template) (Szklarz and Halpert 1997). Roughly, the same secondary structures are identified, but we found  
5 divergences in SRS location between their model and those derived from the present approach. SRS4 and SRS5 match well, but SRS2 is shifted (divergence in the position of helix F along the sequence), while SRS1 (helix B'), SRS3 (helix G) and SRS6 (sheet  $\beta$ 4) are more notably displaced. The loops connecting the secondary structures of these SRS significantly disagree. These differences are  
10 likely to issue from a wrong alignment with the crystal P450 structures in the model of Szklarz and Halpert.

#### **Example 2: Determination of the 3D-structure of P450 3A7.**

The model rebuilding of CYP3A7 was performed according to the techniques  
15 described above in example 1 for CYP3A4, except that we used a restrained set of four-template structures, still including the mammalian CYP2C5, in order to test the robustness of the modeling approach. Below are pointed out only the differences in input data and the results relevant to CYP3A7.

#### **20 *Material***

The coordinates of the four P450 crystal structures: P450BM-3 (2hpd), P450eryF (1oxa), P450 51-like from *Mycobacterium tuberculosis* (1e9x) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank and used as initial template for GOK analysis.

25

#### ***Common Structural Blocks (CSB) determination.***

The GOK parameters were adjusted recursively to values ranging from 10 to 30° ( $\alpha$ -mesh) and 1 to 3 ( $\alpha$ -margin in mesh units). Occasionally, the  $\alpha$ -mesh value was pushed up to 60° to refine some local structured loops (DE loop, HI loop) or short  
30 helices (such as J'). 27 CSBs have been identified. New CSBs were detected: the block 7\* (between blocks 6 and 7A), the block 7B\* (between 7B and 8) and the block 7C (between 7B\* and 8). For the different CSBs, mp-rms value ranged between 0.12 and 4.57 Å in average.

The best alignment found of CYP3A7 on CSBs is shown in **Figure 1**. On the 459 residues comprised in the model structure (the protein was rebuilt depleted of its first 44 residues from the N-terminal domain), 337 residues were found located in CSBs, i.e. 73% of residues belong to structurally conserved regions of the four-  
5 template set.

#### ***Constraints derivation and rebuilding***

With a larger cutoff (12 Å), we obtained around 73000 distance constraints, and 900 dihedral constraints.

- 10 The residue covalently linked to the heme group is at position 442 in the sequence of the protein (**Figure 1**).

#### ***Description of the CYP3A7 model***

- The four-template approach generated converging models, possessing the same  
15 fold. The PROCHECK analysis for structure quality assessment for the lowest energy models showed 74.4% of their non-glycine and non-proline residues with  $\phi$ ,  $\psi$  conformation in the most favoured regions of the Ramachandran plot (core region), 18.2% in additional allowed regions, and 4.7% in the generously allowed regions. 2.7% (11 residues) had their  $\phi$ ,  $\psi$  conformation in disallowed regions. The  
20 total number of residues in the model is 459; which 407 are non-glycine and non-proline residues, and number of residues in the native sequence is 503.

- A closer inspection of the structure, and after the results of dynamics docking experiments (see below), revealed that several hydrogen bonds can hinder the main access to the active site. Thus, key residues that are likely to be involved in the  
25 recognition and admission of the substrate are **Q79; F102; R105; R106; F108; F248; F304 and E374**, and additionally **C98 and C377 (Figure 4B)**. More specifically, R105, R106, Q79 and E374 can establish mutual hydrogen bonds in one of the access channels, and are thus involved in the access of the substrate towards the active site.

30

#### **Example 3: Docking Strategy**

Our aim in this example was to obtain the different positions of the known substrates of CYP3A in the active site, consistent with the oxidation sites and

biochemical differences among the CYP3A isoforms. Considering the fact that the heme-binding site is deeply buried in the protein structure, and thus the selection and the pathway of the substrates within the enzyme structure are strongly dependent on the various possibilities of structure opening, we implemented a special approach more appropriate to flexible structures, hereafter referred as “restrained dynamics docking” or “soft-restrained dynamics docking”. This technique employs constrained molecular dynamics simulations, where the only constraints are heme-substrate distances. The successive steps are:

10 ***Conversion of the PDB XPLOR file in PDB for SYBYL file***

The optimized structures with XPLOR (PDB format) are visualized with the SYBYL 6.6 software (Tripos Inc.), which implies a conversion of the file (atoms types correction) so as to make it compatible and exploitable in the constrained dynamics which will be performed with SYBYL.

15

***Stabilization of the P450 3A4 model generated under XPLOR***

Then, we do aggregate N°1 (in the meaning of SYBYL) with all the NC $\alpha$ CO atoms of the peptide backbone of the protein. The structure is relaxed with a dynamic of 10ns at 100K followed by a minimization of 100 steps. Agregate N°1 is then deleted.

20

We do aggregate N°2 constituted of the protein C $\alpha$  only. The protein relaxation is reiterated with a dynamic of 10 ns at 100K and a minimization of 100 steps. Agregate N°2 is then deleted.

The all protein is then relaxed with a first dynamic of 1ns at 100K, followed by a dynamic of 1ns at 200K and a dynamic of 10ns at 300K. We terminate with a minimization of 100 steps.

25

***Restrained dynamics docking of the substrate (example: testosterone)***

We do aggregate N°3 constituted of all atoms outside a sphere of 20Å around the C $\alpha$  of residues constituting the heart of the B' loop. We also add heminic iron to this aggregate.

30

The substrate is placed inside the protein, at around 30Å from the heminic iron and next to SRS1 and SRS5 sites. The substrate is placed so that the constraints between

the hemic iron and the substrate backbone go between SRS1, SRS5 and SRS3. Thus, for testosterone docking, we establish 4 distance constraints (limit below 3Å, above 10Å) between hemic iron and C3, C8, C10 and C13 carbons with a constraint of 2 kcal/Å on the entire structure so as to avoid to favour the approach of one part of the substrate more than the other.

We begin to perform a dynamic without constraints of the entire system at 20 K during 2ns to stabilize the system, then we perform a dynamic under constraints at 20 K during 5ns. We observe that the substrate worms between SRS1, SRS3 et SRS5 to reach a position at the vicinity of hemic iron. We terminate with a dynamic without constraints at 300 K to relax the system and we realize a minimization of 1000 steps.

### ***Results***

We found that the testosterone molecule is positioned at the vicinity of hemic iron in such way that the C6 of testosterone be at 4.9Å of the iron, which is compatible with the hydroxylation of this compound to give 6β-hydroxy-testosterone (Figure 4A).

Minimizations and dynamics with the SYBYL software are performed with the Tripos force field following the parameters: dielectric constant equal to 1 and distance-dependent, minimization method of POWELL, a minimum gradient of 0.05kcal.mol<sup>-1</sup>.Å<sup>-1</sup>, electrostatics charges calculated according to the Gasteiger-Hückel method, and a NB cutoff of 8.0Å (non-bond energies). The energetic diagram of dynamic docking of testosterone is shown in Figure 5.

### ***Interest of this docking strategy:***

Most P450 isozymes recognize only one substrate (for specific catalysis in a metabolic pathway), or a very limited number of substrates, all chemically closely related. At the contrary, CYP 3A isozymes are known to recognize a large palette of substrates, and are also capable of multiple binding in the active site, up to three molecules in the vicinity of the heme, according to the model developed by Hosea et al. 2000. Multiple pharmacophoric behavior (Ekins et al. 2003), as well as allosteric or synergistic effects, characterize the members of this P450 subfamily.

The docking strategy described above can be easily extended to different binding and metabolism scenario.

For example, the docking of two or three testosterone molecules, or of two testosterone molecules and one alpha-naphthoflavone molecule ( $\alpha$ NF) can be simulated in the following manner:

- In a first step, a testosterone molecule is dynamically docked under constraints, and then released of its constraints to freely evolve in the active site and find a first bound equilibrium position.
- In a next step, an external testosterone is presented, at the same entrance of the protein structure or in the vicinity of another access channel, and then dynamically docked under constraints. The system first evolves under constraints applied to the second molecule, and can be released for a subsequent free MD simulation of the two molecules bound in the active site. One can see the first bound molecule (testosterone or another substrate) to be re-oriented under the effect of the second docking, simulating a situation of cooperativity.
- Similarly, the second molecule docked can be different from the first bound, *e.g.* . a first testosterone bound to the active site followed by the docking of an  $\alpha$ NF molecule, or the reverse situation.
- One can combine of course the possibilities: for example, two molecules (identical or of different chemical nature) are docked following the two steps above, and then, after stabilization around an equilibrium position, a third molecule is introduced under constraints, and then released from its constraints to let the system evolving towards a favorable energetic conformational state. In this way, two  $\alpha$ NF and one testosterone or one  $\alpha$ NF and two testosterone can be docked.
- Of course, not only substrates can be docked, but also inhibitors. The docking procedure above can help to measure the potential inhibitory power of a molecule, for example a compound comprising an imidazole group. A first step would include a standard constrained dynamic docking of the potential inhibitor, followed by a free MD simulation (constraints are released when the inhibitor is in the active site), or by a specifically-constrained MD simulation where the imidazole group is confined in the vicinity of the hemic iron by using an additional distance constraint Fe-imidazole. In a following step, a second substrate is dynamically docked under constraints from the exterior, and one can determine in what

conditions the second molecule can chase the first one from its binding position. The strength of the additional constraint can be a measurement of the inhibitory potential.

Correspondingly, the exit pathway of the metabolites can be explored by simulating  
5 the exit of the molecule bound to the active site, using either free MD simulation (if the chemical nature of the transformed molecule allows an energetical instability), or using inverted constraints, *i.e.* soft distance constraints (between an external point and the bound molecule) that help to expel out the metabolite. Additionally, the best exit pathway can be deduced from the most favored energy profiles.

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